MassBank User's Manual

Version 2.3, 9 December 2010

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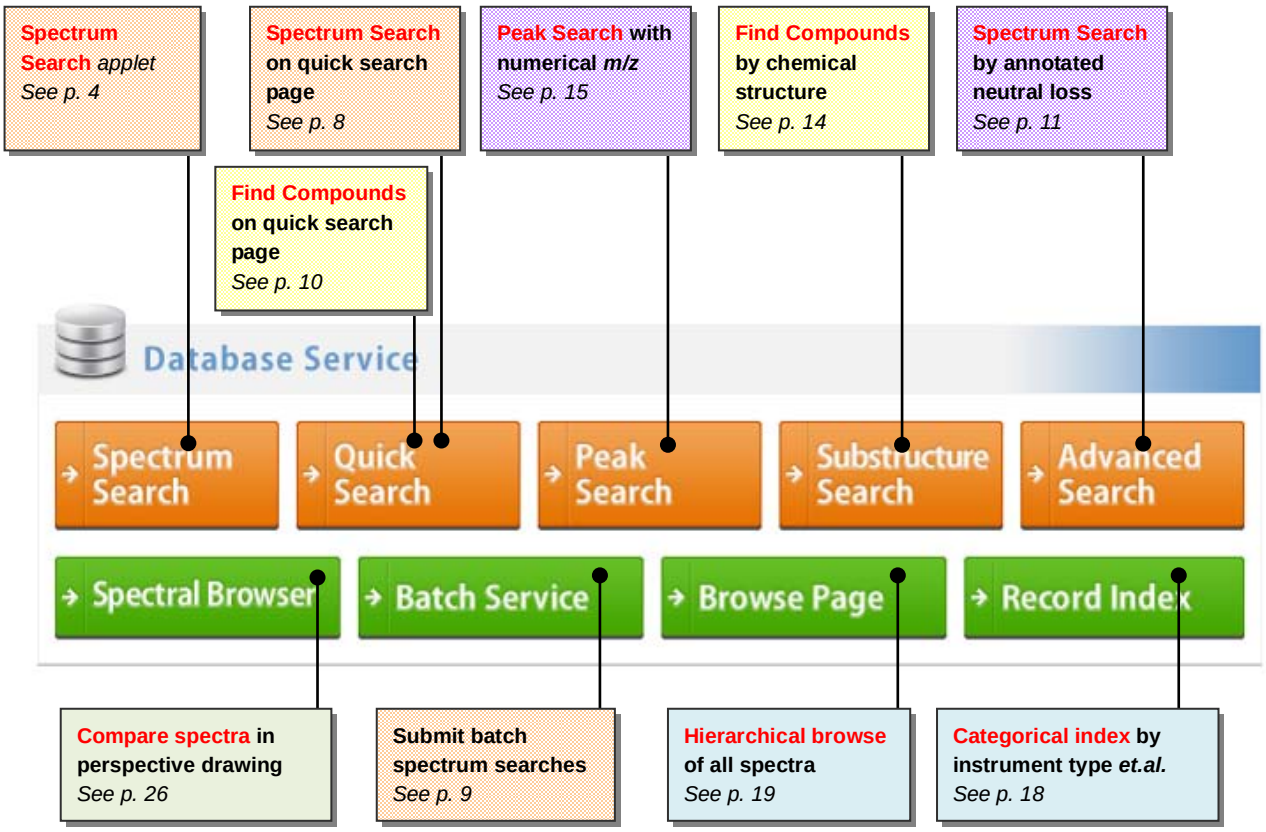
1. Introduction

This manual mainly describes the operation of the MassBank database services.

1.1 Overview of the Database Services

MassBank provides the following database services.



1.2 System Requirements

Below are the system requirements for using the MassBank database services.

(1) Web Browser

We recommend using Internet Explorer 6 or higher, or Firefox 2 or higher as your browser.

(2) Web Browser Settings

Make sure that your Web browser is configured as follows.

[1] JavaScript execution enabled

[2] Popups enabled

- See the page below for instructions on how to check this (URL to allow: http://www.massbank.jp)
  http://www.microsoft.com/japan/seminar/help/popup.mspx

(3) Install Java runtime environment

The Java Runtime Environment (JRE) Version 5 or higher must be installed.

- You can use the page below to check your installation status and download Java.
  http://www.java.com/en/download/

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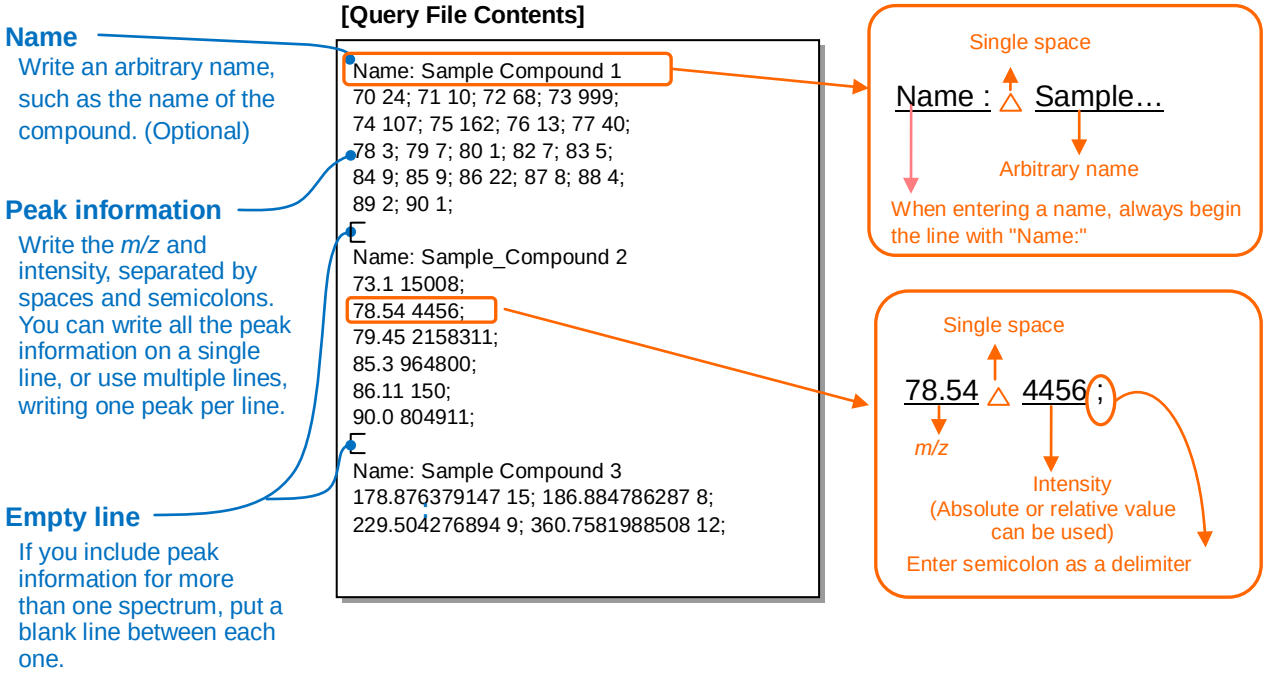
2. Searching for Similar Spectra

2.1 Spectrum Search Applet

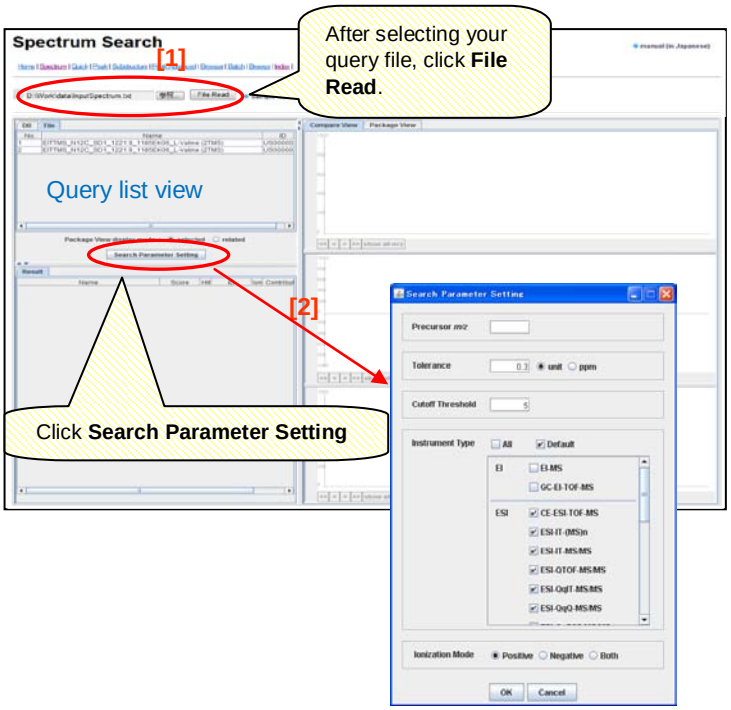
Spectrum Search enables you to perform GUI-based spectrum searches in a Web browser. Spectra in the MassBank similar to one provided by the user as a query are retrieved and displayed in a list. It is also possible to graphically compare the query spectrum with the retrieved spectrum.

(1) Prepare the query file

When performing a spectrum search with the applet, you must prepare a query file in one of the following formats. A sample can be downloaded from http://www.massbank.jp/sample/sample.zip


[Query File Contents]
Name
Write an arbitrary name, such as the name of the compound. (Optional)
Peak information
Write the m/z and intensity, separated by spaces and semicolons. You can write all the peak information on a single line, or use multiple lines, writing one peak per line.
Empty line
If you include peak information for more than one spectrum, put a blank line between each one.
Name: Sample Compound 1
70 24; 71 10; 72 68; 73 999;
74 107; 75 162; 76 13; 77 40;
78 3; 79 7; 80 1; 82 7; 83 5;
84 9; 85 9; 86 22; 87 8; 88 4;
89 2; 90 1;
Name: Sample_Compound 2
73.1 15008;
78.54 4456;
79.45 2158311;
85.3 964800;
86.11 150;
90.0 804911;
Name: Sample Compound 3
178.876379147 15; 186.884786287 8;
229.504276894 9; 360.7581988508 12;
Single space
Name : Sample…
Arbitrary name
When entering a name, always begin the line with "Name:"
Single space
78.54 4456;
m/z
Intensity
(Absolute or relative value can be used)
Enter semicolon as a delimiter

(2) Load the query and configure the search parameters



Search Parameter Setting Window

[1] Load the query file

Click **Browse**, and select the query file you have prepared. Click **File Read** to load the file. After the file finishes loading, a list of queries appears.

[2] Set the search parameters

Click **Search Parameter Setting**. The Setting window opens.

Settings

- **Precursor *m/z*** :
  Precursor ion specified by *m/z*
- **Tolerance**:
  m/z error range
- **Cutoff Threshold**:
  Relative intensity threshold
- **Instrument Type**:
  Type of instrument
- **Ionization Mode**:
  Mode of ionization

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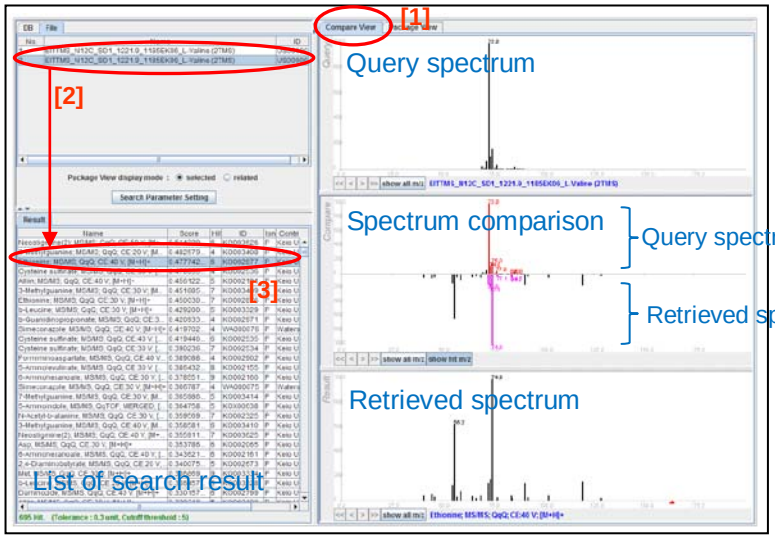
(3) Perform the search

Compare View: Compare query and retrieved spectrums one to one.



[1] Select "Compare View"

Click to select.
It is selected by default.

[2] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectrums are retrieved.

[3] Select a retrieved spectrum

Click to select any spectrum in the list of search result.

Package View: Compare query and retrieved spectrums one to many.

[1] Select "Package View"

Click to select.

[2] Select package view display mode

Click "**selected**" or "**related**".

[3] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectrums are retrieved.

[4] Select a retrieved spectrum

Click to select any spectrum in the list of search result. If you chose "**selected**" in step 2, then you can hold down Ctrl + Shift to select multiple rows. If you chose "**related**" in step 2, then only one row can be selected.

Different Display Modes in Package View

There are two display modes in Package View.

selected

Multiple spectrums can be selected from the list of search results. The selected spectrums and the query spectrum are shown in a tiled view.

related

Only one spectrum can be selected from the list of search results. The selected spectrum, a spectrum with different collision energy than the selected spectrum (detected automatically), and the query spectrum are displayed in tiled view.

Peak Color in Spectrum Comparison Window

In the spectrum comparison windows in Compare View and Package View, matching peaks can be distinguished by color.

Matching m/z on query peak / *Peak*	Perfect Match	Match within Error Margin
Query Spectrum	**Red**	**Red**
Retrieved Spectrum	**Red**	**Pink**

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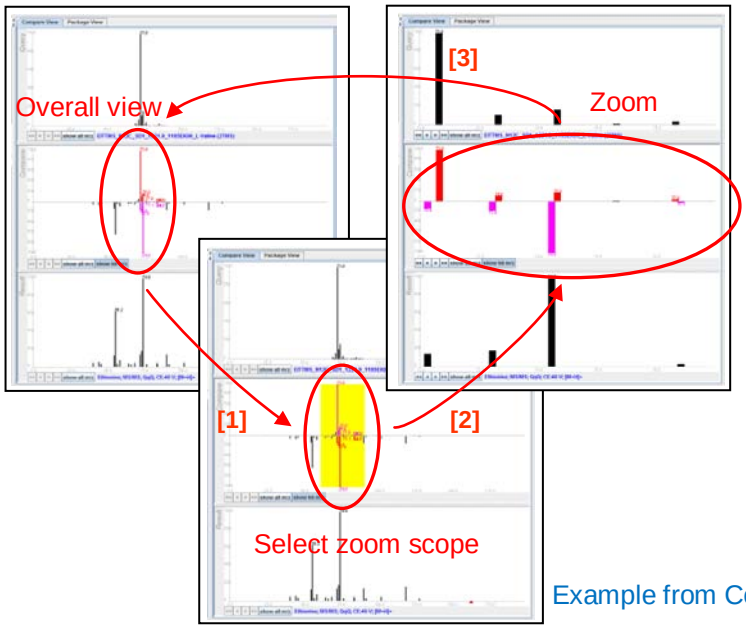
<<Handy Feature 1: Spectrum Zoom>>



Example from Compare View

[1] Select location to zoom

Drag from the location of the start of the zoom.

[2] Set zoom position

Drop to set the location on the spectrum to zoom.

[3] End zoom

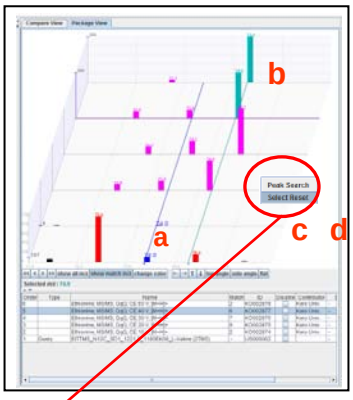
Double click on the spectrum.

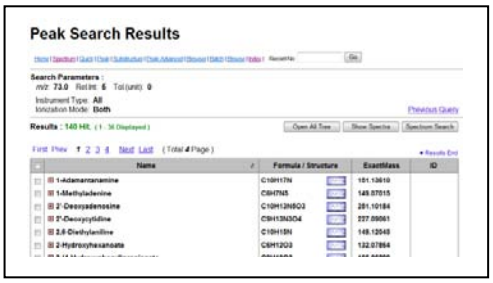
Note: You can also zoom on spectrums from the Package View.

<<Handy Feature 2: Peak Manipulation>>

Example from Compare View

Example from Package View





Peak Search Results Window

a. Highlight peak

Place the cursor over a peak. It is highlighted in blue, and the *m/z* and intensity values appear.

b. Select peak

Click on a peak. It is rendered in blue to indicate that it is selected. Up to 6 peaks can be selected.

c. Search for peaks

If you right click while one or more peaks are selected, a menu appears, and "Peak Search" can be selected. The peak search begins immediately after selection.

d. Cancel peak selection

When you right click on the spectrum, a menu appears. Chose **"Select Reset"**.

Peak Rendering Color

Highlighted: Blue

Selected: Light blue

Highlighting and Selecting Peaks in Package View

When multiple spectrums are displayed in Package View, you can highlight or select the peaks in any spectrum. When you do so, if there is a peak in another spectrum with a perfectly matching *m/z*, then that peak is also highlighted or selected.

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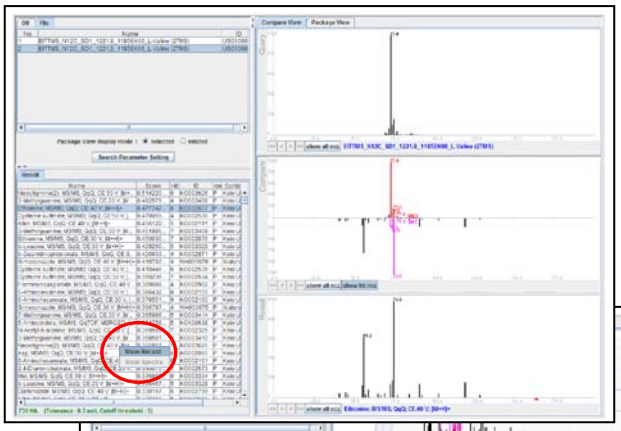
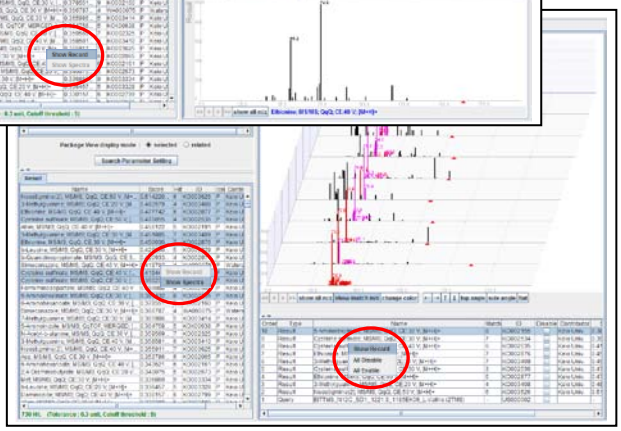
<<Handy Feature 3: Show Record>>

Example from Compare View

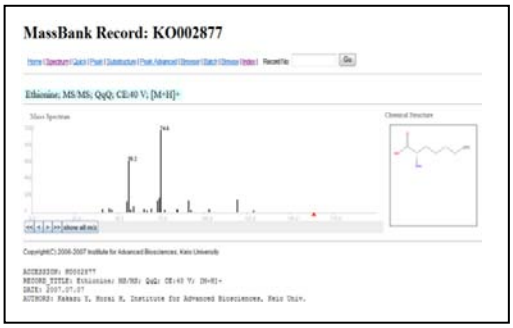




Example from Package View

a. Show record

When you right click with one spectrum selected, the "**Show Record**" command appears on the menu. Select this to view details about the spectrum.



b. Show multiple spectra

When you right click with two or more spectra selected, the "**Show Spectra**" command appears on the menu. Select this to display multiple spectra in tiled view.

<<Handy Feature 4: Spectrum Manipulation>>

Spectrum Manipulation Buttons in Compare View

<<、<、>、>>	Move display location (only when zoomed on spectrum)
show all *m/z*	Display *m/z* values of all peaks
show hit *m/z*	Display *m/z* values of matching peaks

Spectrum Manipulation Buttons in Package View

<<、<、>、>>	Move display location (only when zoomed on spectrum)
show all *m/z*	Display *m/z* values of all peaks
show match *m/z*	Display *m/z* values of matching peaks
change color	Change color of entire spectrum
←、→、↑、↓	Change angle (manual manipulation)
top angle	Change angle (top perspective)
side angle	Change angle (side perspective)
flat	Change angle (all spectrums in flat view)

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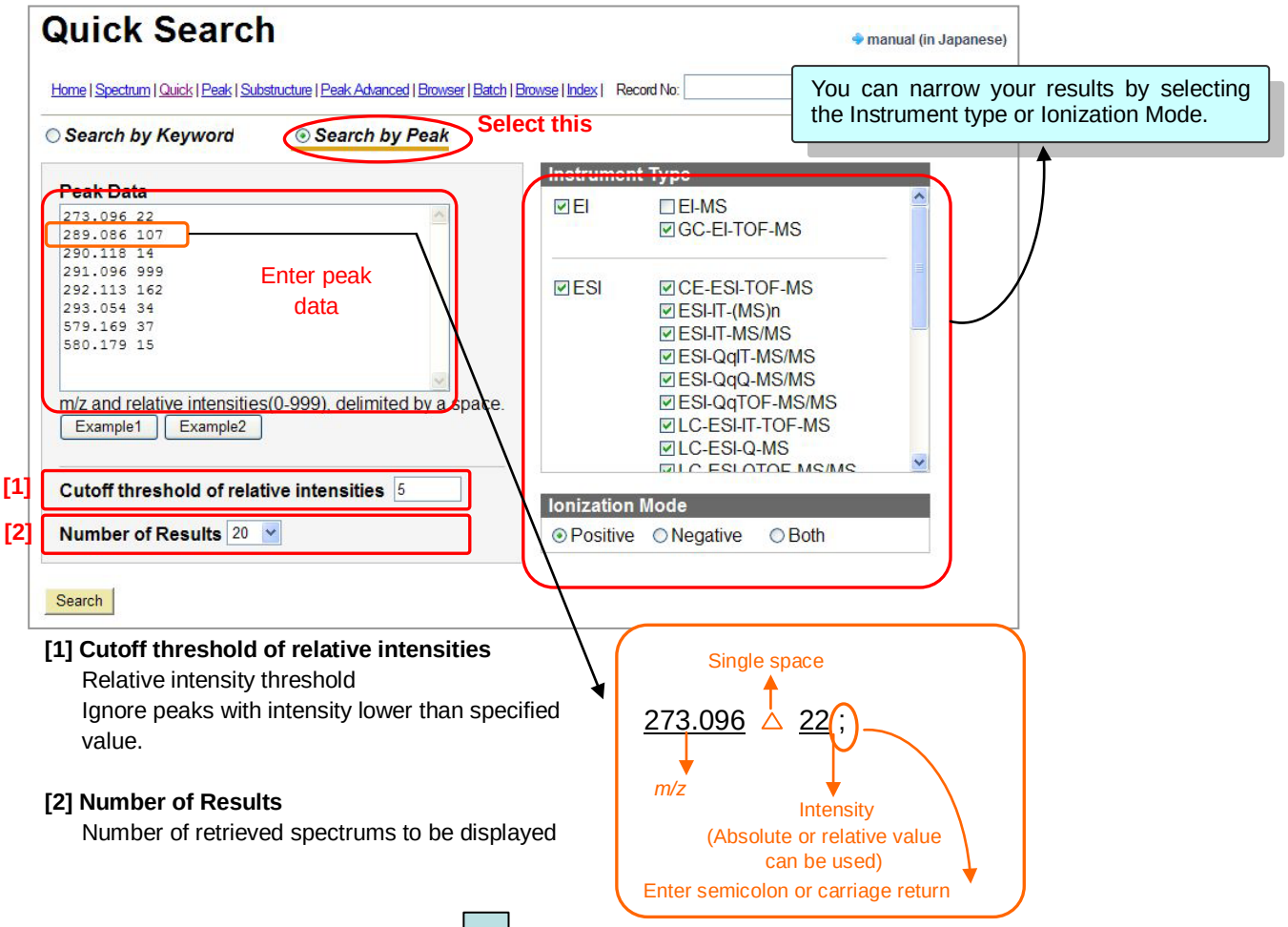
2.2 Spectrum Search on Quick Search Page

The Quick Search feature allows you to search for similar spectrums just using simple input.

>> Enter Search Parameters



[1] Cutoff threshold of relative intensities

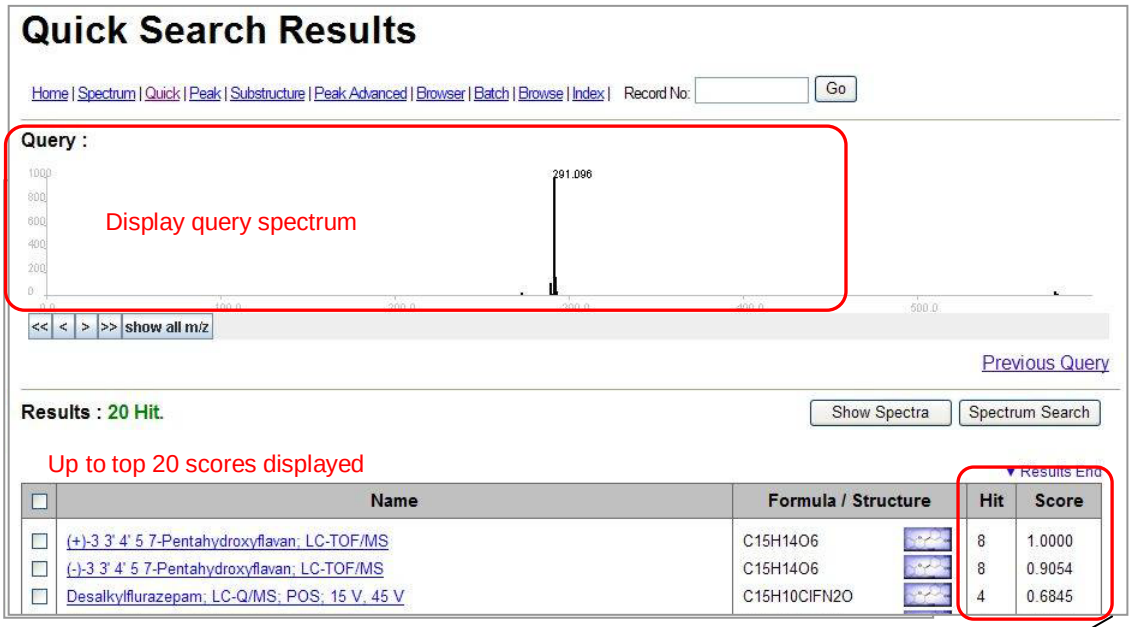
Relative intensity threshold

Ignore peaks with intensity lower than specified value.

[2] Number of Results

Number of retrieved spectrums to be displayed

>> Display Search Results



Hit: Number of peaks in the retrieved spectrums matched to those in a query data

Score: Similarity score of retrieved spectrum to a query data

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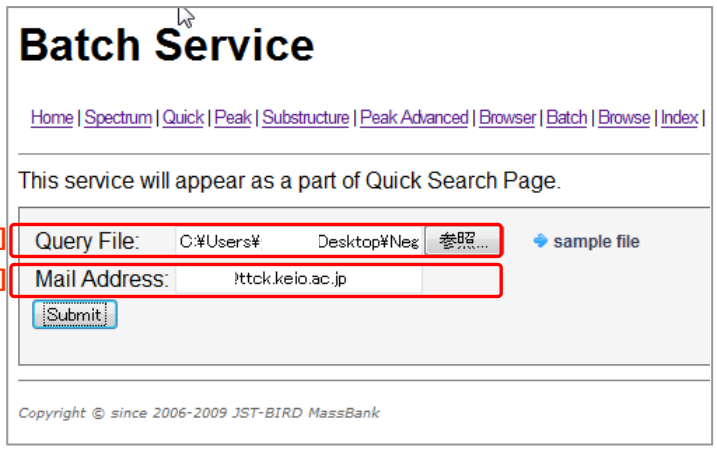
2.3 Conduct Batch Spectrum Searches

Batch Service conducts a batch spectrum search, and emails you the results.

Use this in such cases as when you would like to search for a large number of spectra.



[1] Load the query file

Prepare a query file with the same format as the one described in "2.1 (1) Spectrum Search Applet". Click **Browse**, and select the query file you have prepared.

[2] Enter email address

Enter the email address to which you would like the search results sent.

Click **Submit** to perform the batch query. A message appears indicating that the query has been accepted.

Batch Service
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser
[2009/09/25 18:41:51]
Your batch search is accepted.
The results will be sent to ynihei@ttck.keio.ac.jp later.

Search results are sent to the specified address by e-mail. The following files are attached to the e-mail: (1) Search Results; and (2) Summary of Results.

(1) Search Results (Text Format)

***** MassBank Batch Service Results *****

Request Date: 2010/10/15 14:07:51 JST
Instrument Type:
CE-ESI-TOF-MS,ESI-IT-(MS)n,ESI-IT-MS/MS,ESI-QTOF-MS/MS,ESI-QqIT-MS/MS,ESI-QqQ-MS/MS,ESI-QqTOF-MS/MS,LC-ESI-FT-MS,LC-ESI-IT-MS/MS,LC-ESI-IT-TOF-MS,LC-ESI-Q-MS,LC-ESI-QTOF-MS/MS,LC-ESI-QqQ-MS/MS,LC-ESI-TOF-MS
Ion Mode: Negative

Query 1
Name: Scan530 — **Name of a query spectrum**
Hit: 37

Top 20 List — **LIst of search results (at most 20 high-scored spectra)**

Accession	Title	Formula	Mass	Score	Hit		
KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	133.03751	0.3545	2		
KNA00487	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	133.03751	0.3104	2		
KNA00752	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	105.04259	0.3041	2		
KNA00542	cis-Aconitate; LC-ESI-FT-MS; NEG	C6H6O6	174.01644	0.2955	2		
KNA00475	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	105.04259	0.2942	2		
KNA00628	L-Glutamine; LC-ESI-FT-MS; NEG	C5H10N2O3	146.06914	0.2911	2		
KNA00728	L-Homoserine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2904	2		
KNA00812	Citrate; LC-ESI-FT-MS; NEG	C6H8O7	192.027	0.2885	2		
KNA00820	3-Phospho-D-glycerate; LC-ESI-FT-MS; NEG	C3H7O7P	185.99294	0.2844	2		
KNA00554	L-Homoserine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2823	2		
KNA00538	sn-Glycerol 3-phosphate; LC-ESI-FT-MS; NEG	C3H9O6P	172.01367	0.2756	2		
KNA00527	(S)-Malate; LC-ESI-FT-MS; NEG	C4H6O5	134.02152	0.2746	2		
KNA00648	L-Threonine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2716	2		
KNA00736	L-Asparagine; LC-ESI-FT-MS; NEG	C4H8N2O3	132.05349	0.2713	2		
KNA00808	cis-Aconitate; LC-ESI-FT-MS; NEG	C6H6O6	174.01644	0.2673	2		
KNA00491	L-Glutamine; LC-ESI-FT-MS; NEG	C5H10N2O3	146.06914	0.2663	2		
KNA00483	L-Asparagine; LC-ESI-FT-MS; NEG	C4H8N2O3	132.05349	0.2650	2		
KNA00696	4-Hydroxy-L-proline; LC-ESI-FT-MS; NEG	C5H9NO3	131.05824	0.2646	2		
KNA00546	D-Gluconic acid; LC-ESI-FT-MS; NEG	C6H12O7	196.0583	0.2616	2		
KNA00530	2-Oxoglutarate; LC-ESI-FT-MS; NEG	C5H6O5	146.02152	0.2587	2		

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(2) Summary of Results (HTMLformat)

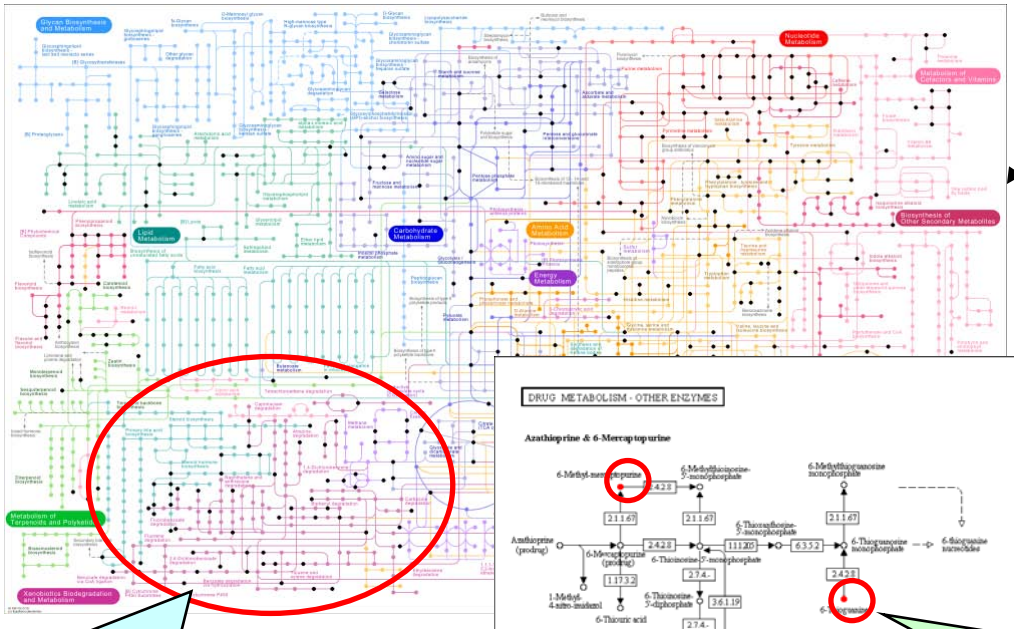
Summary Of Batch Service Results

Request Date : 2010/10/15 14:07:51 JST

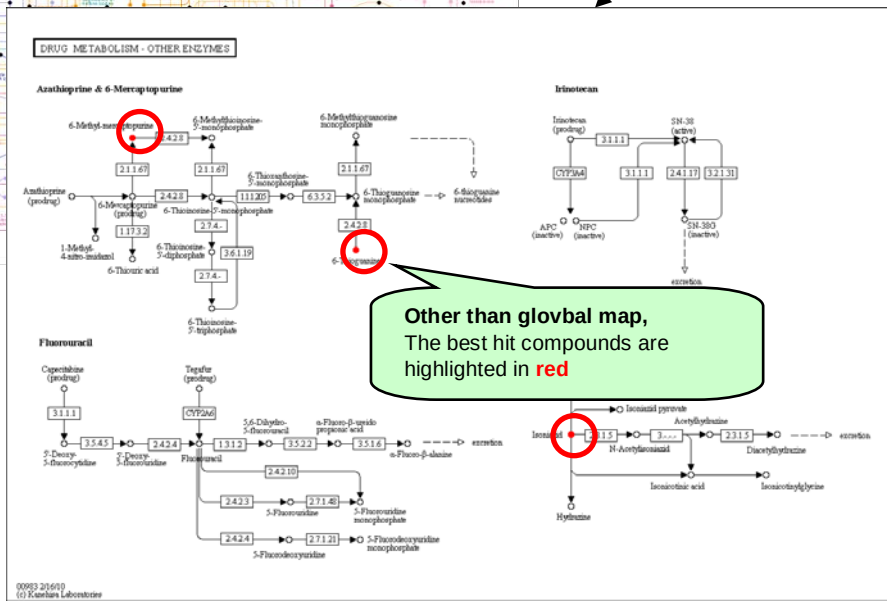
Instrument Type : CE-ESI-TOF-MS,ESI-IT-(MS)n,ESI-IT-MS/MS,ESI-QTOF-MS/MS,ESI-QqIT-MS/MS,ESI-QqQ-MS/MS,ESI-QqTOF-MS/MS,LC-ESI-FT-MS,LC-ESI-IT-MS/MS,LC-ESI-IT-TOF-MS,LC-ESI-Q-MS,LC-ESI-QTOF-MS/MS,LC-ESI-QqQ-MS/MS,LC-ESI-TOF-MS
Ion Mode : Negative

List of the best hit for each query

No.	Query Name	Score	MassBank ID	Record Title	Formula	KEGG ID	Colored Pathway Maps			
							MAP1	MAP2	MAP3	MAP4
1	Scan530	0.3545	KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	C00049	map01100(28)	-	-	-
2	Scan531	0.9999	KO001625	Propiolate; MS/MS; QqQ; CE:10 V; [M-H]-	C3H2O2	C00804	-	-	-	-
3	Scan532	0.2593	KNA00475	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	C00065	map01100(28)	-	-	-
4	Scan534	0.3524	KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	C00049	map01100(28)	-	-	-
5	Scan535	0.9999	KO001625	Propiolate; MS/MS; QqQ; CE:10 V; [M-H]-	C3H2O2	C00804	-	-	map00640(1)	-
6	Scan538	No Hit Record								
7	Scan539	0.0751	UT002896	Phosphatidylethanolamine alkenyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84NO7P	-	-	-	-	-
8	Scan540	0.4198	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
9	Scan542	No Hit Record								
10	Scan543	0.1230	UT002896	Phosphatidylethanolamine alkenyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84NO7P	-	-	-	-	-
11	Scan544	0.4294	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
12	Scan546	0.0876	UT002244	Phosphatidylserine 18:1-22:0 / 20:0-20:1; LC-MS/MS; Orbitrap; m/z: 844.61; [M-H]-; RT: 51.49; Exp: 2	C47H90NO8P	-	-	-	-	-
13	Scan547	0.5831	PR050557	Acetylsalicylic acid; ESI-QTOF-MS/MS; MERGED; [M-H]-	C9H8O4	-	-	-	-	-
14	Scan548	0.1290	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
15	Scan550	0.3157	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
16	Scan551	0.4388	WA000541	Pentobarbital sodium salt; LC-Q/MS; NEG; 30 V	C11H17N2NaO3	-	-	-	-	-
17	Scan552	0.1185	TY000116	Baicalin; LC-ESI-IT-MS/MS; [M-H]-	C21H18O11	-	-	-	-	-
18	Scan554	0.2940	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
19	Scan555	0.1109	UT002896	Phosphatidylethanolamine alkenyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84NO7P	-	-	-	-	-
20	Scan556	0.5934	PR050557	Acetylsalicylic acid; ESI-QTOF-MS/MS; MERGED; [M-H]-	C9H8O4	-	-	-	-	-
21	Scan558	No Hit Record								
22	Scan559	0.1074	UT002896	Phosphatidylethanolamine alkenyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84NO7P	-	-	-	-	-
23	Scan560	0.1286	PB004142	Kaempferol; MS/MS; QqQ; CE:35 eV; [M-H]-	C15H10O6	C05903	map01100(28)	-	-	-
24	Scan562	No Hit Record								
25	Scan563	0.2191	UT002452	Phosphatidylserine 18:0-20:1 / 18:1-20:0; LC-(MS)3; Orbitrap; m/z: 816.57/729.15; [M-H]-/[M-Ser]-; RT: 43.92; Exp: 2	C45H86NO9P	-	-	-	-	-
26	Scan564	0.4069	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
27	Scan566	No Hit Record								
28	Scan567	0.0201	MT000095	taurochenodeoxycholate; MS/MS; IT; m/z: 498.3; [M-H]-	C26H45NO6S	C05465	-	-	-	map00121(1)
29	Scan568	0.4064	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-



Click a link, then the pathway map is displayed. In the pathway map, the best hit compounds of all queries are highlighted



In **global map** (map:01100), the best hit compounds are highlighted in **black**.

Other than glovbal map, The best hit compounds are highlighted in **red**

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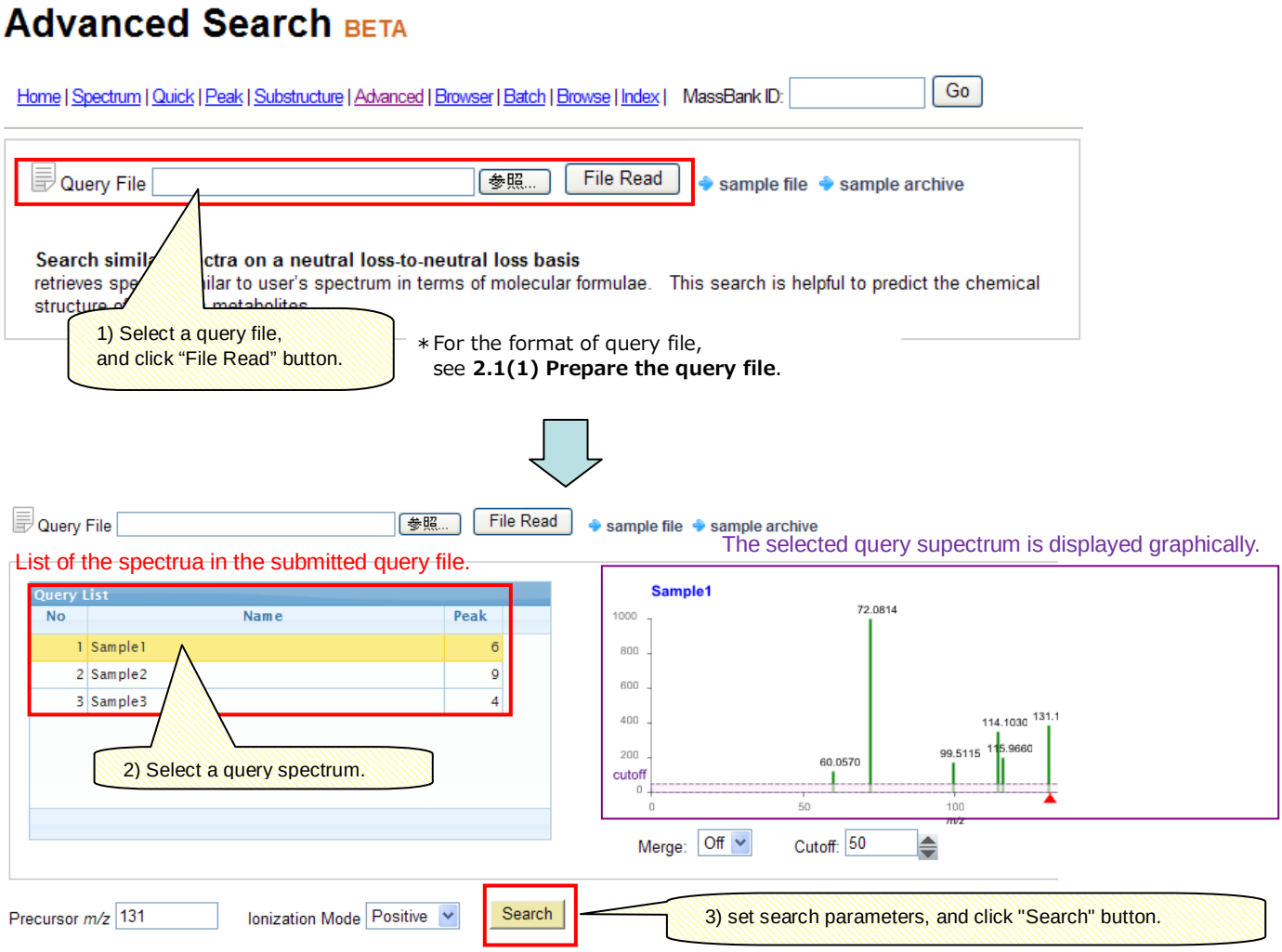
2.4 Spectral Search by Annotated Neutral Loss

In Advanced Search, an unknown compound is identified by a MS^n spectrum by the similarity of formulae of neutral loss molecules. Even if there is not a spectrum of the correct answer in MassBank, you can obtain valuable information for compound identification by investigating some common characteristics among structures of high-ranking compounds because the similarity of structures among compounds is inherited to the similarity of detected neutral losses among spectra of them.

>> Input Search Parameters


Advanced Search BETA
Home | Spectrum | Quick | Peak | Substructure | Advanced | Browser | Batch | Browse | Index | MassBank ID: Go
Query File 参照... File Read sample file sample archive
1) Select a query file, and click "File Read" button.
*For the format of query file, see 2.1(1) Prepare the query file.
List of the spectrua in the submitted query file.
The selected query supectrum is displayed graphically.
Query List
No Name Peak
1 Sample1 6
2 Sample2 9
3 Sample3 4
2) Select a query spectrum.
Sample1
72.0814
60.0570
99.5115
114.1030
131.1
cutoff
Merge: Off Cutoff: 50
Precursor m/z 131 Ionization Mode Positive Search
3) set search parameters, and click "Search" button.

– Search Parameters –

・**Precursor *m/z*** :
m/z of the precursor is set automatically. The default value is *m/z* of the right most peak in the selected query spectrum whose relative intensity is more than or equal to 50 %. **If the default value is not adequate, please revise it manually.**

・**Ionization Mode** :
Select "Positive" or "Negative".

・**Merge** :
You can merge several spectra in to a query and use it as the query spectrum. When "On" is selected, a checkbox appears to each spectrum in the left sided list for specifying spectra to merge.

・**Cut off** :
Ignore every peak whose relative intensity is less than the specified value.

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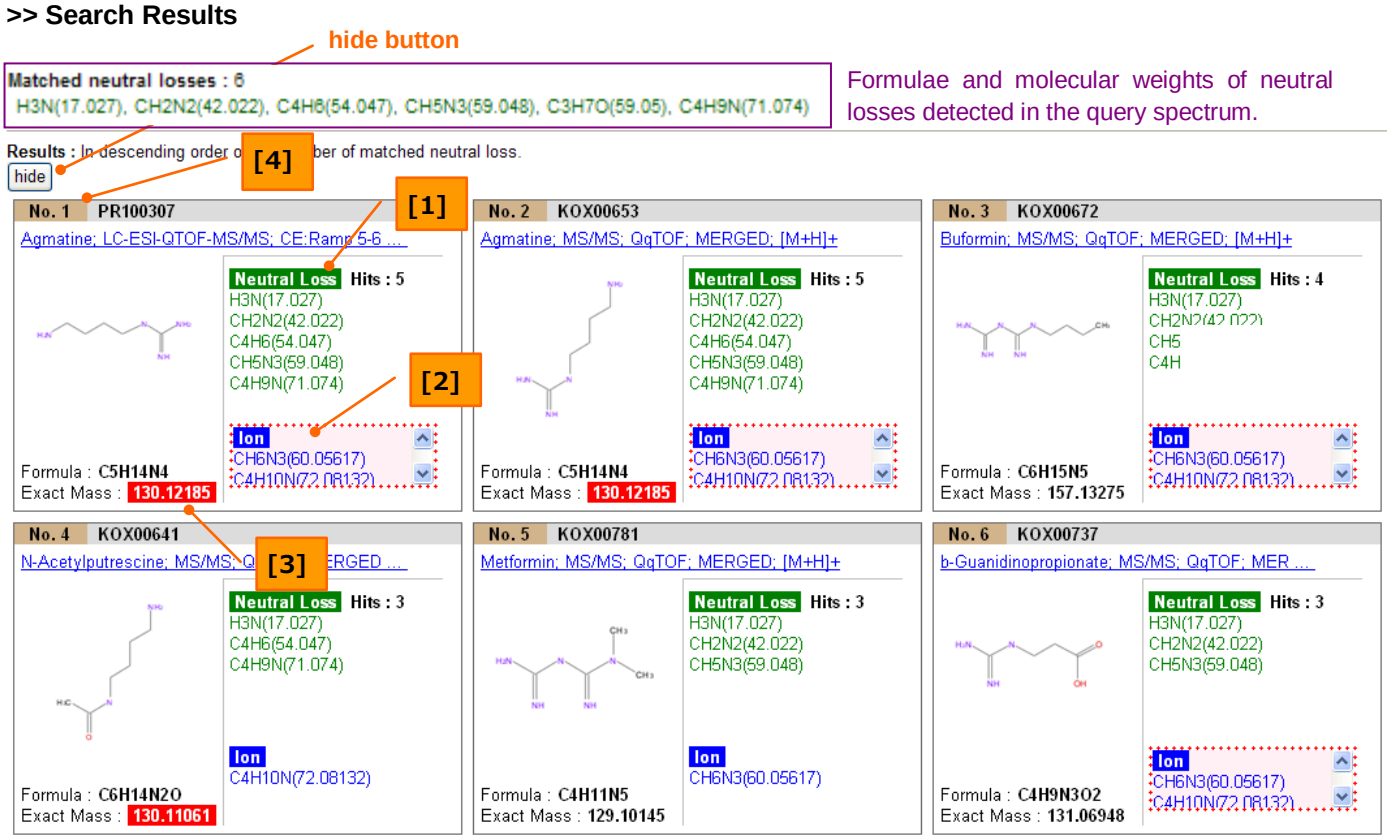
>> Search Results



At most 30 hits of MassBank Records are displayed

[1]**Neutral Loss** : Number and formulae of neutral losses matched to ones detected in the query spectrum.
・・・Search results are sorted in descending order of the number of the neutral losses.

[2]**Ion** : Formulae of ions matched to ones detected in the query where the integer value of *m/z* is between 50 and 99.
・・・A, Surrounded by a red dotted line: The result has the most detected ions of 30 hits in the page.
(No.1, 2, 3 and 6 in this example. They have two ions which is the most in this page.)
B, Black on gray: The number of ions is equal to zero.
* Click hide button (in front of No.1), then these results become hidden.
C, Message **" NO peaks within *m/z* 50-99 in query."**: There are no peaks in query within the range.
D, Message **"NO matched ions to peaks within *m/z* 50-99 in query."**: There are peaks in query within the range but there are no matched peaks in the search result.

[3]**Exact Mass**
・・・White on red: The value is projected by the precursor *m/z*. The precursor *m/z* is equal to the increment / decrement of the exact mass when the ionization mode is "positive" / "negative" (130+1 = 131 in this example).
・・・White on gray: There is 50 or more difference between the exact mass and the precursor *m/z*.

[4]**Ranking**
・・・The search results are sorted in descending order of the number of the matched neutral losses in [1].
In the case of a tie, they are sorted in ascending order of the difference between the exact mass in [3] and the projected one by the precursor *m/z*. See the above [3] for the details of the prediction using the ionization mode.

Support Conditions on Equality or Similarity of Chemical Structure

・Higher ranking. Especially in the case of [2] A.
・Not in the case of [2] B.
・In the case of "white on red" in [3]. It is mandatory for similarity of chemical structure.

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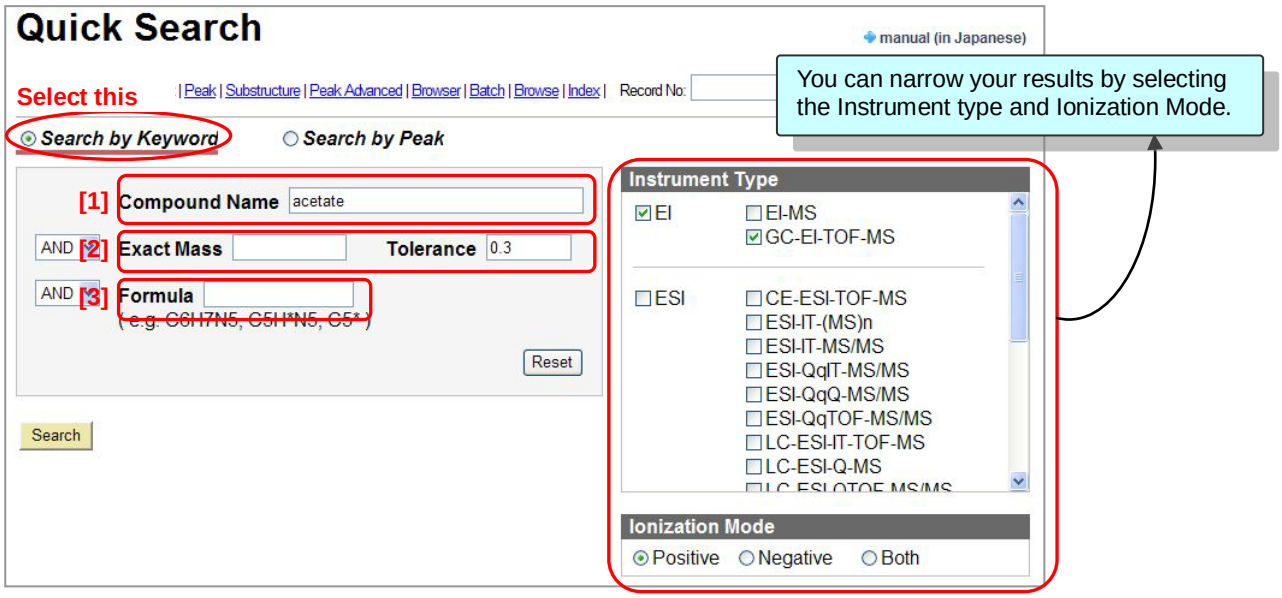
3. Compound Search

3.1 Find Compounds on Quick Search Page

The Quick Search feature allows you to search for compounds by compound name, molecular formula, etc.

>> Enter Search Parameters



[1] Compound Name

Enter the compound name. Names with substring matches on the string you entered are retrieved.

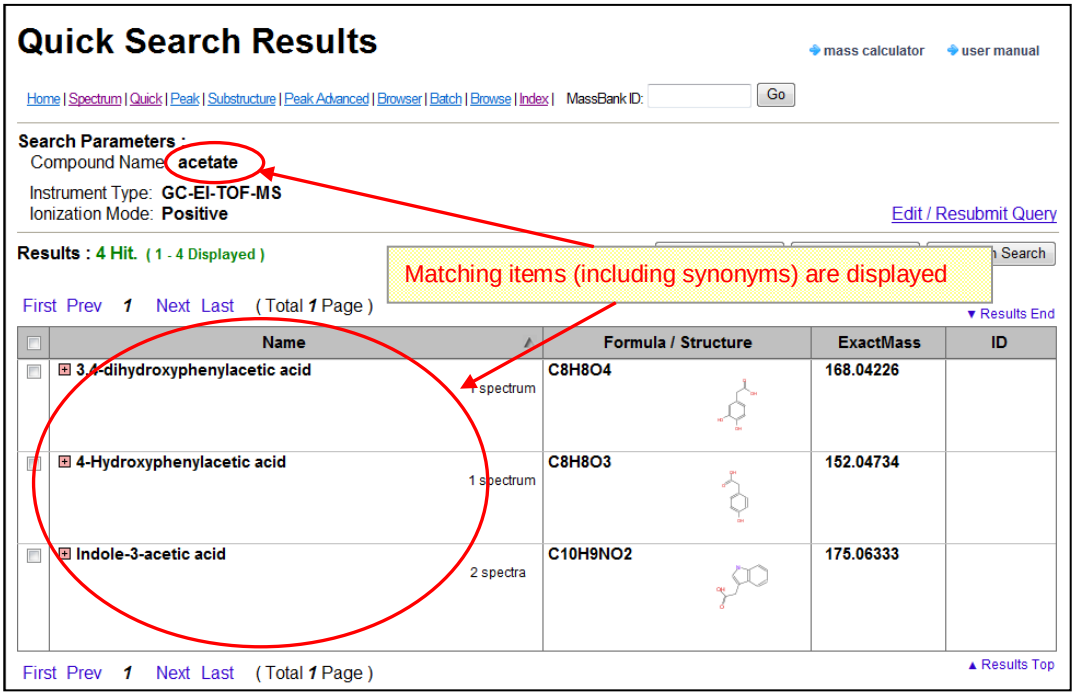
[2] Exact Mass/Tolerance

Enter the exact mass and error tolerance.

[3] Formula

Enter the molecular formula of the compound. Enter the formula starting with "C", followed by "H", and then the other letters in alphabetical order. Add wildcards ("*") to find partial matches.
Example: C5H*N5

>> Display Search Results



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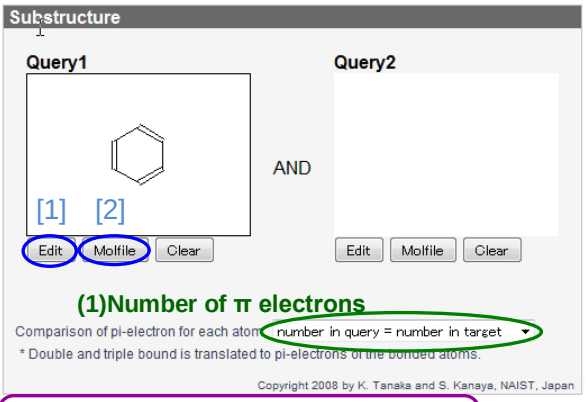
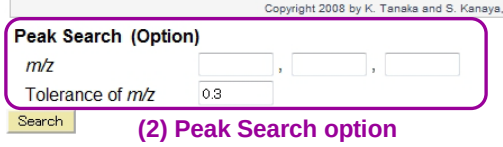
3.2 Find Compounds by Chemical Structure

The Substructure Search enables you to find compounds including the specified chemical structure.

>> Enter Search Parameters





(2) Peak Search option

(1) Number of π electrons

- Query structure = target structure (default)
- Query structure ≤ target structure
- No comparison

(2) Peak Search option

Specify *m/z* values to perform peak search at same time.

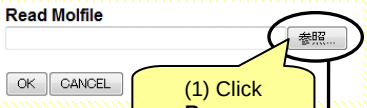
You can also narrow your results by selecting the Instrument type or Ionization Mode.

Enter query structure

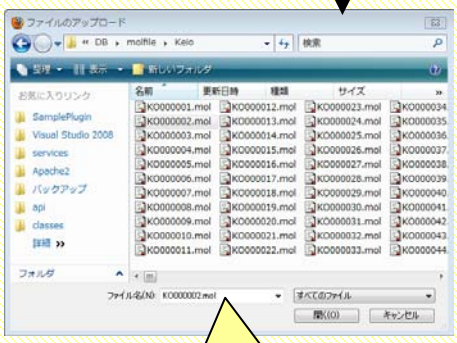
[1] Write in editor

Or:

[2] Load Molfile



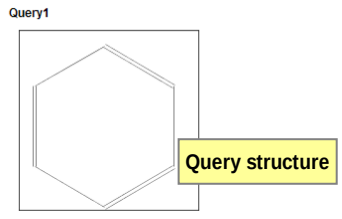
(1) Click **Browse**

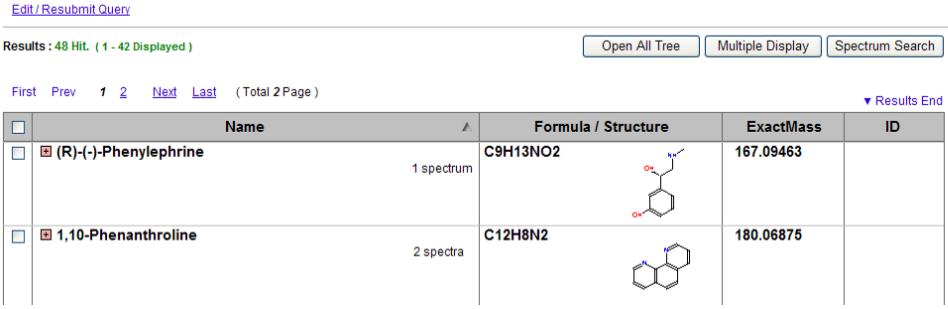


(2) Select a file

The loaded structure formula can be modified in the editor as well.

>> Display Search Results





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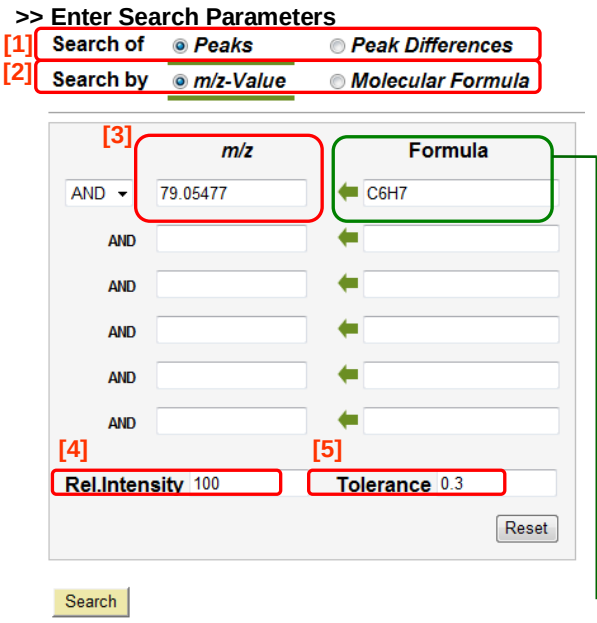
4. Peak Search

4.1 Peak Search by *m/z* values

Peak Search enables you to find peaks by specifying the *m/z* or *m/z* difference as numerical values.



[1] Search of "Peaks" or "Peak Differences"
- "Peaks": search of the *m/z* value.
- "Peak Differences": search of the *m/z* differences.

[2] Search by "*m/z*-Value" or "Molecular Formula"
Select ""m/z-Value" for Peak Search by *m/z* values.

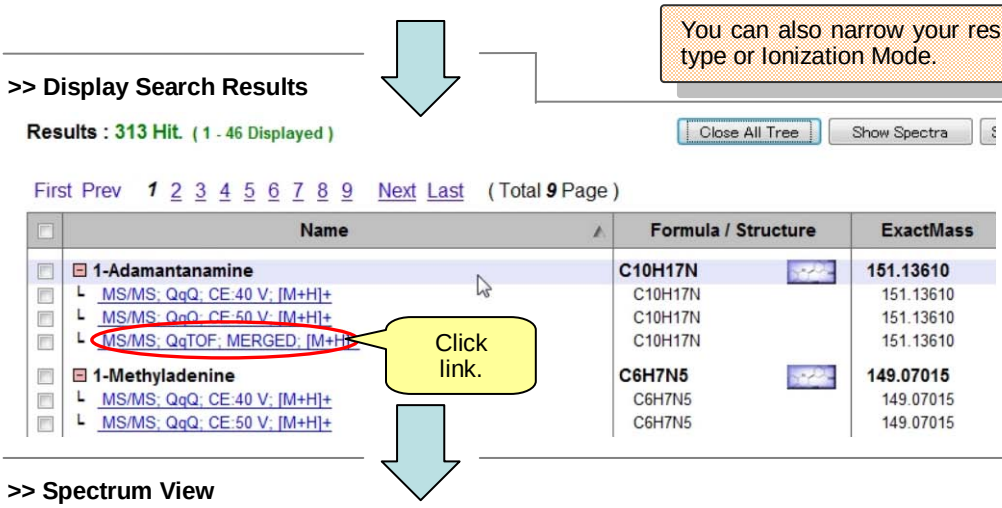
[3] *m/z*
Specify the peak *m/z* value. You can specify up to 6, and connect them via AND or OR conditions.

[4] Rel. Intensity
Ignore peaks with intensity lower than specified value. Specify a relative intensity from 1 to 999.

[5] Tolerance
Specify the *m/z* error range.

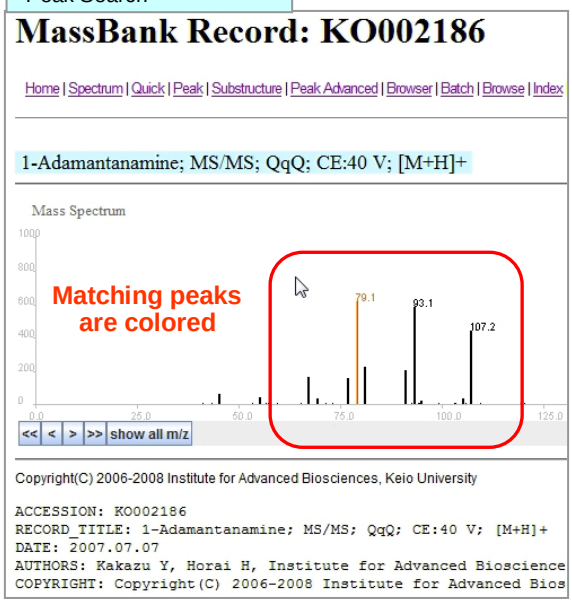
Converting from molecular formula to *m/z*
Enter a molecular formula the exact calculated mass in the *m/z* text box. The exact calculated mass is truncated to 5 decimal place.

You can also narrow your results by selecting the Instrument type or Ionization Mode.

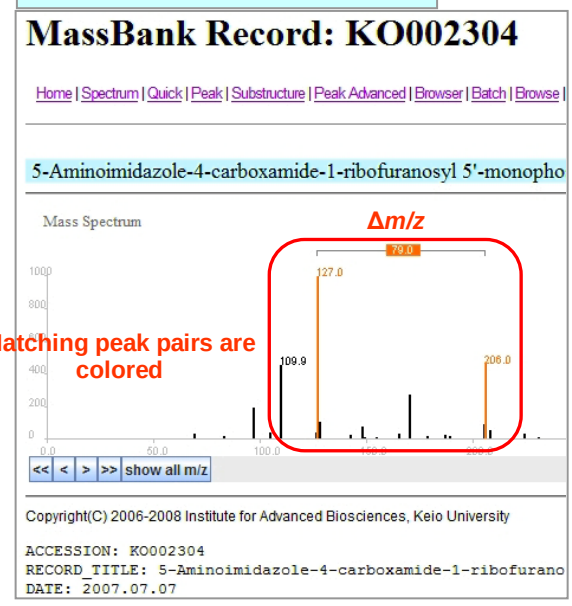


>> Spectrum View

Peak Search


MassBank Record: KO002186
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index
1-Adamantanamine; MS/MS; QqQ; CE:40 V; [M+H]+
Mass Spectrum
Matching peaks are colored
79.1
93.1
107.2
<< < > >> show all m/z
Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University
ACCESSION: KO002186
RECORD_TITLE: 1-Adamantanamine; MS/MS; QqQ; CE:40 V; [M+H]+
DATE: 2007.07.07
AUTHORS: Kakazu Y, Horai H, Institute for Advanced Bioscience
COPYRIGHT: Copyright(C) 2006-2008 Institute for Advanced Bios

Peak Difference Search



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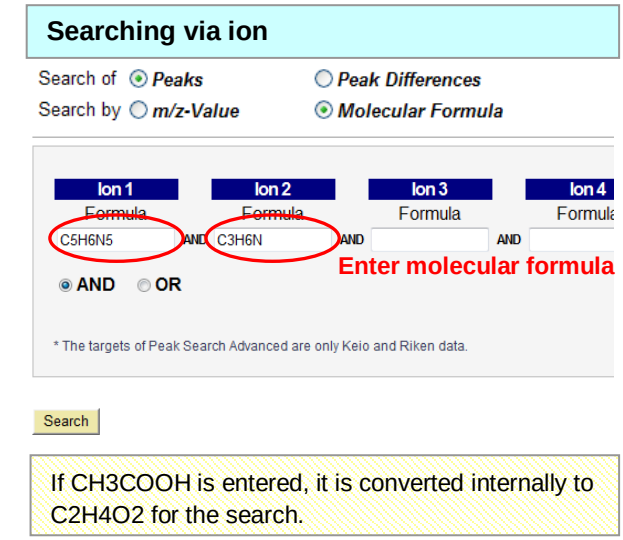
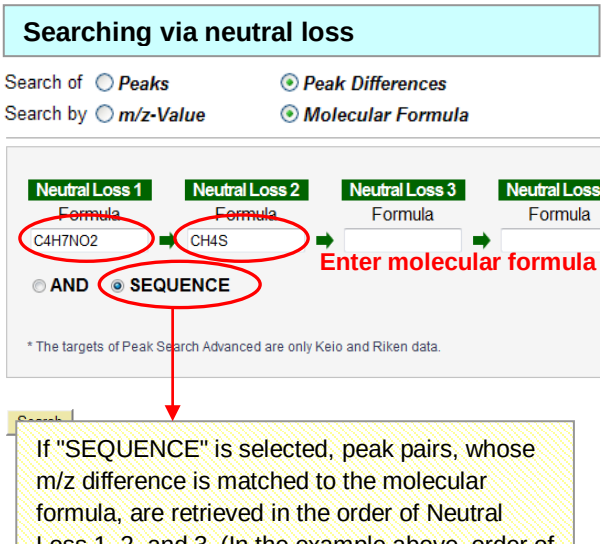
4.2 Peak Search with Molecular Formulas

Peak Search Advanced enables you to find peaks by specifying an ion or neutral loss by molecular formulas instead of a numerical *m/z* values.

>> Enter Search Parameters

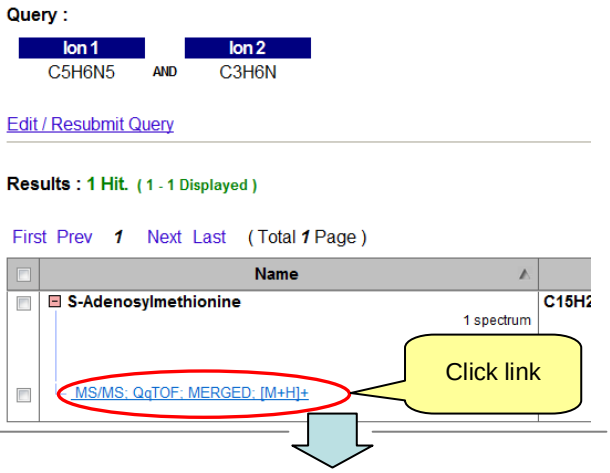


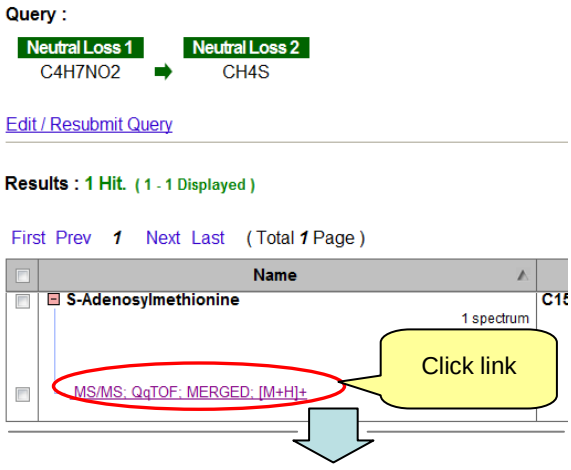
If CH3COOH is entered, it is converted internally to C2H4O2 for the search.


Searching via neutral loss
Search of Peaks Peak Differences
Search by m/z-Value Molecular Formula
Neutral Loss 1 Formula
Neutral Loss 2 Formula
Neutral Loss 3 Formula
Neutral Loss Formula
C4H7NO2
CH4S
AND SEQUENCE
Enter molecular formula
* The targets of Peak Search Advanced are only Keio and Riken data.

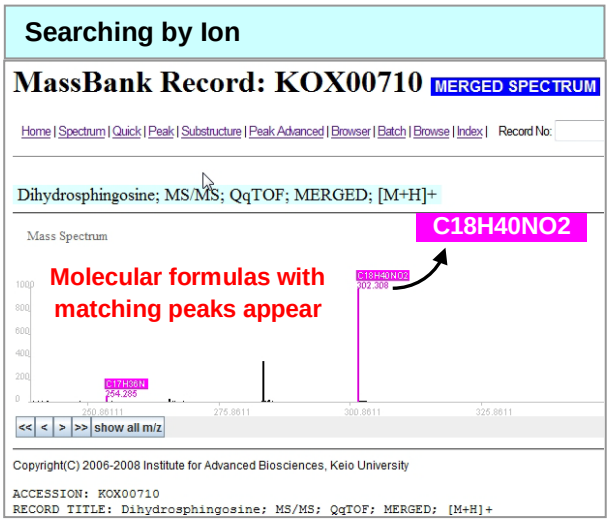
If "SEQUENCE" is selected, peak pairs, whose m/z difference is matched to the molecular formula, are retrieved in the order of Neutral Loss 1, 2, and 3. (In the example above, order of CH4H7NO2, then CH4S)

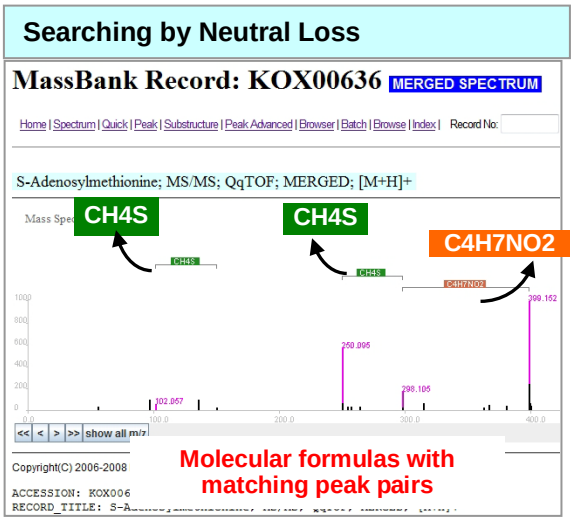
>> Display Search Results


Query :
Ion 1 C5H6N5 AND Ion 2 C3H6N
Edit / Resubmit Query
Results : 1 Hit. (1 - 1 Displayed)
First Prev 1 Next Last (Total 1 Page)
Name
S-Adenosylmethionine
C15H2
1 spectrum
MS/MS; QqTOF; MERGED; [M+H]+
Click link


Query :
Neutral Loss 1 C4H7NO2 Neutral Loss 2 CH4S
Edit / Resubmit Query
Results : 1 Hit. (1 - 1 Displayed)
First Prev 1 Next Last (Total 1 Page)
Name
S-Adenosylmethionine
1 spectrum
MS/MS; QqTOF; MERGED; [M+H]+
Click link

>> Spectrum View


Searching by Ion
MassBank Record: KOX00710 MERGED SPECTRUM
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No:
Dihydrosphingosine; MS/MS; QqTOF; MERGED; [M+H]+
Mass Spectrum
C18H40NO2
Molecular formulas with matching peaks appear
show all m/z
Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University
ACCESSION: KOX00710
RECORD_TITLE: Dihydrosphingosine; MS/MS; QqTOF; MERGED; [M+H]+

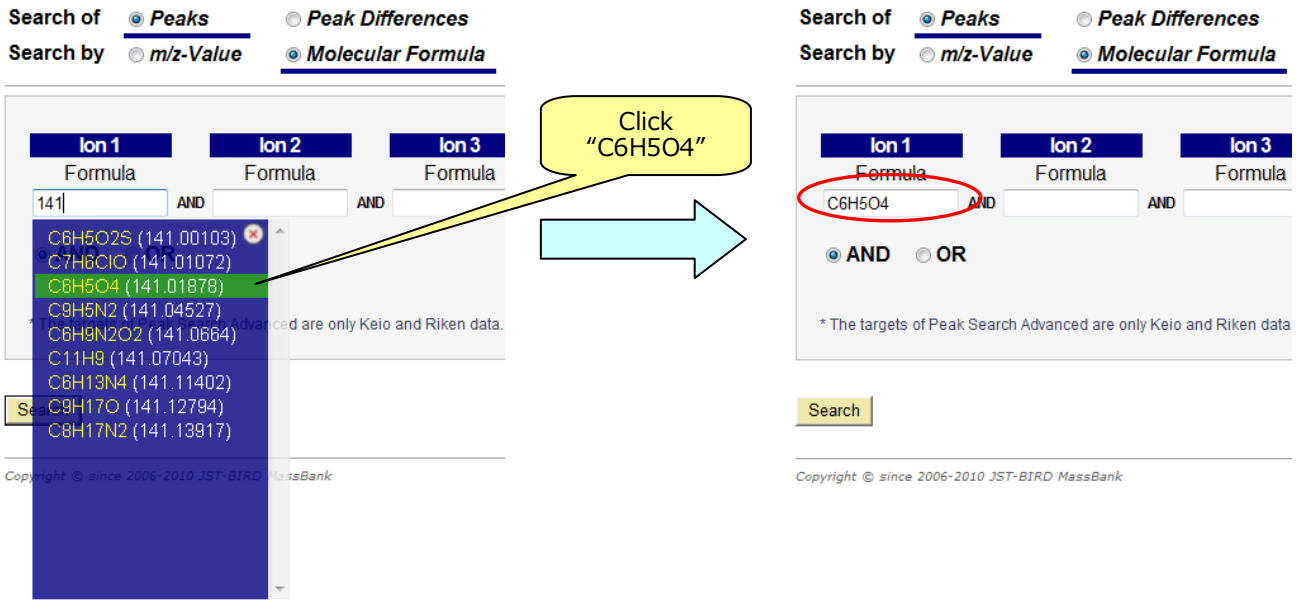

Searching by Neutral Loss
MassBank Record: KOX00636 MERGED SPECTRUM
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No:
S-Adenosylmethionine; MS/MS; QqTOF; MERGED; [M+H]+
CH4S
CH4S
C4H7NO2
show all m/z
Copyright(C) 2006-2008
Molecular formulas with matching peak pairs

Copyright© 2006-2010 JST-BIRD MassBank

＊Assist in the Input of Molecular Formulas

When *m/z* values instead of molecular formulas are entered in the "Formula" boxes, a list of candidate molecular formulas, whose exact masses are close to the entered *m/z* values, is shown in the pull-down menu.

Following example shows a case when a value, 141, was entered in a Formula box on the "Search of Peaks" and "Search by Molecular Formula" mode.



Pull-down menu shows a list of the molecular formulas, whose exact masses is starting from a values of 141. No molecular formula such as 140.9 are listed because prefix string match algorithm is applied.

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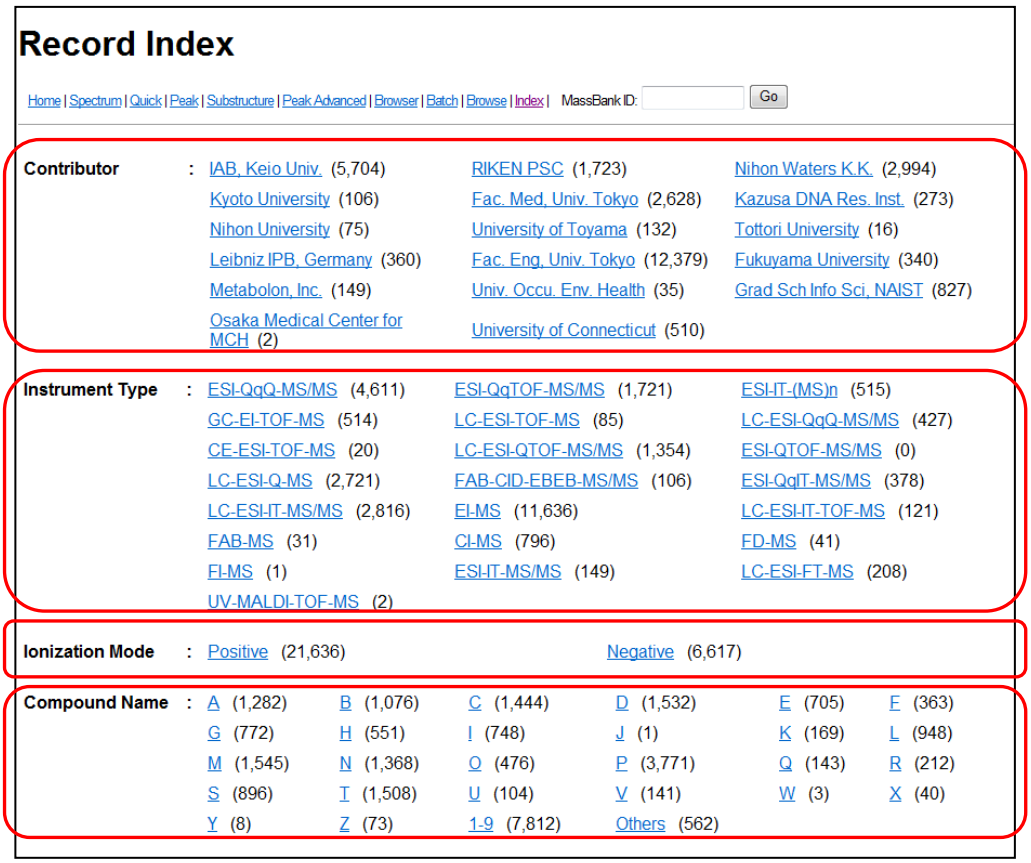
5. Browsing All Data

5.1 Categorical Index

In Record Index, all data is categorized into contributor, instrument type, ionization mode and compound name categories. Click a link in this page, then the whole data in the category is displayed in the same format as other search results.


Record Index
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | MassBank ID: Go
Contributor : IAB, Keio Univ. (5,704) RIKEN PSC (1,723) Nihon Waters K.K. (2,994)
Kyoto University (106) Fac. Med, Univ. Tokyo (2,628) Kazusa DNA Res. Inst. (273)
Nihon University (75) University of Toyama (132) Tottori University (16)
Leibniz IPB, Germany (360) Fac. Eng, Univ. Tokyo (12,379) Fukuyama University (340)
Metabolon, Inc. (149) Univ. Occu. Env. Health (35) Grad Sch Info Sci, NAIST (827)
Osaka Medical Center for MCH (2) University of Connecticut (510)
Instrument Type : ESI-QqQ-MS/MS (4,611) ESI-QqTOF-MS/MS (1,721) ESI-IT-(MS)n (515)
GC-EI-TOF-MS (514) LC-ESI-TOF-MS (85) LC-ESI-QqQ-MS/MS (427)
CE-ESI-TOF-MS (20) LC-ESI-QTOF-MS/MS (1,354) ESI-QTOF-MS/MS (0)
LC-ESI-Q-MS (2,721) FAB-CID-EBEB-MS/MS (106) ESI-QqIT-MS/MS (378)
LC-ESI-IT-MS/MS (2,816) EI-MS (11,636) LC-ESI-IT-TOF-MS (121)
FAB-MS (31) CI-MS (796) FD-MS (41)
FI-MS (1) ESI-IT-MS/MS (149) LC-ESI-FT-MS (208)
UV-MALDI-TOF-MS (2)
Ionization Mode : Positive (21,636) Negative (6,617)
Compound Name : A (1,282) B (1,076) C (1,444) D (1,532) E (705) F (363)
G (772) H (551) I (748) J (1) K (169) L (948)
M (1,545) N (1,368) O (476) P (3,771) Q (143) R (212)
S (896) T (1,508) U (104) V (141) W (3) X (40)
Y (8) Z (73) 1-9 (7,812) Others (562)
[1]
[2]
[3]
[4]

Each link is followed by the parenthesized number of spectra in the category.

[1] Contributor

Category set of spectrum contributors..

[2] Instrument Type

Category set of instrument types.

[3] Ionization Mode

Category set of ionization modes, *i.e.* positive and negative modes.

[4] Compound Name

Categorized by the first letters of compound names.

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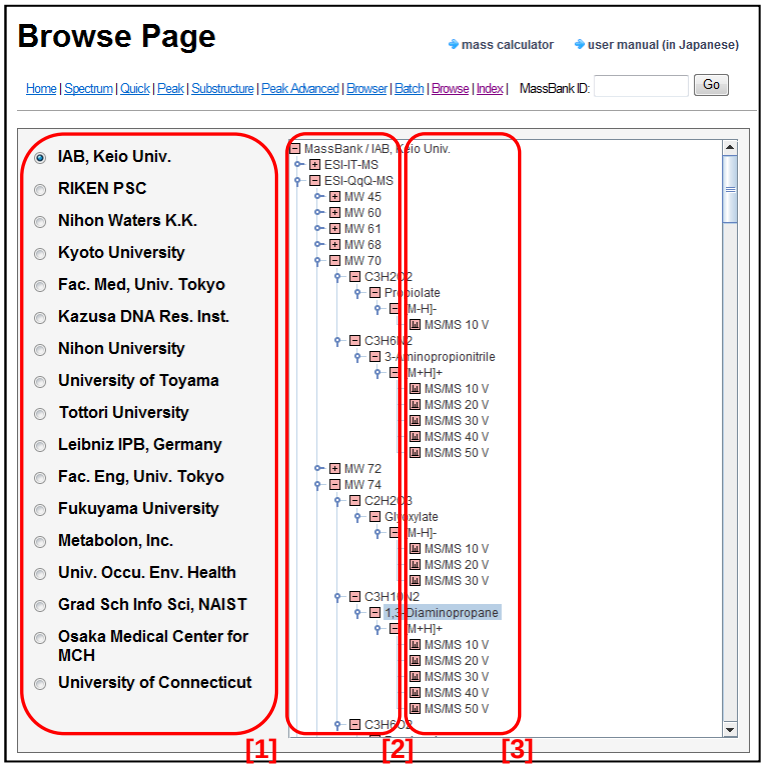
5.2 Hierarchical Browse

In Browse Page, all data are hierarchically displayed for each data provider. You can go up and down the hierarchy (tree) and find a specific data you want.



After selecting a spectrum by clicking, you can select multiple spectra by clicking with Ctrl key or Shift key.
After that, a right button click shows the following popup menu.

[case of single selection]

Click "Show Record", then the details of the MassBank Record are diplayed.

[case of multiple selection]

Click "Multiple Display", then multiple spectra are displayed in tiled view.

[1] Select Provider

Click a radio button, then display the hierarchy of the selected provider is displayed in right hand side.

[2] Browse Tree

: open the lower layer.
: close the lower layer.

[3] Display Spectrum

View detailed MassBank Record: Double click of ; or "Show Record" in popup menu by right button cllick when a spectrum is selected.

Display multiple spectra in a tiled view: "Mutiple Display" in popup menu by right button click when multiple spectra are selected.

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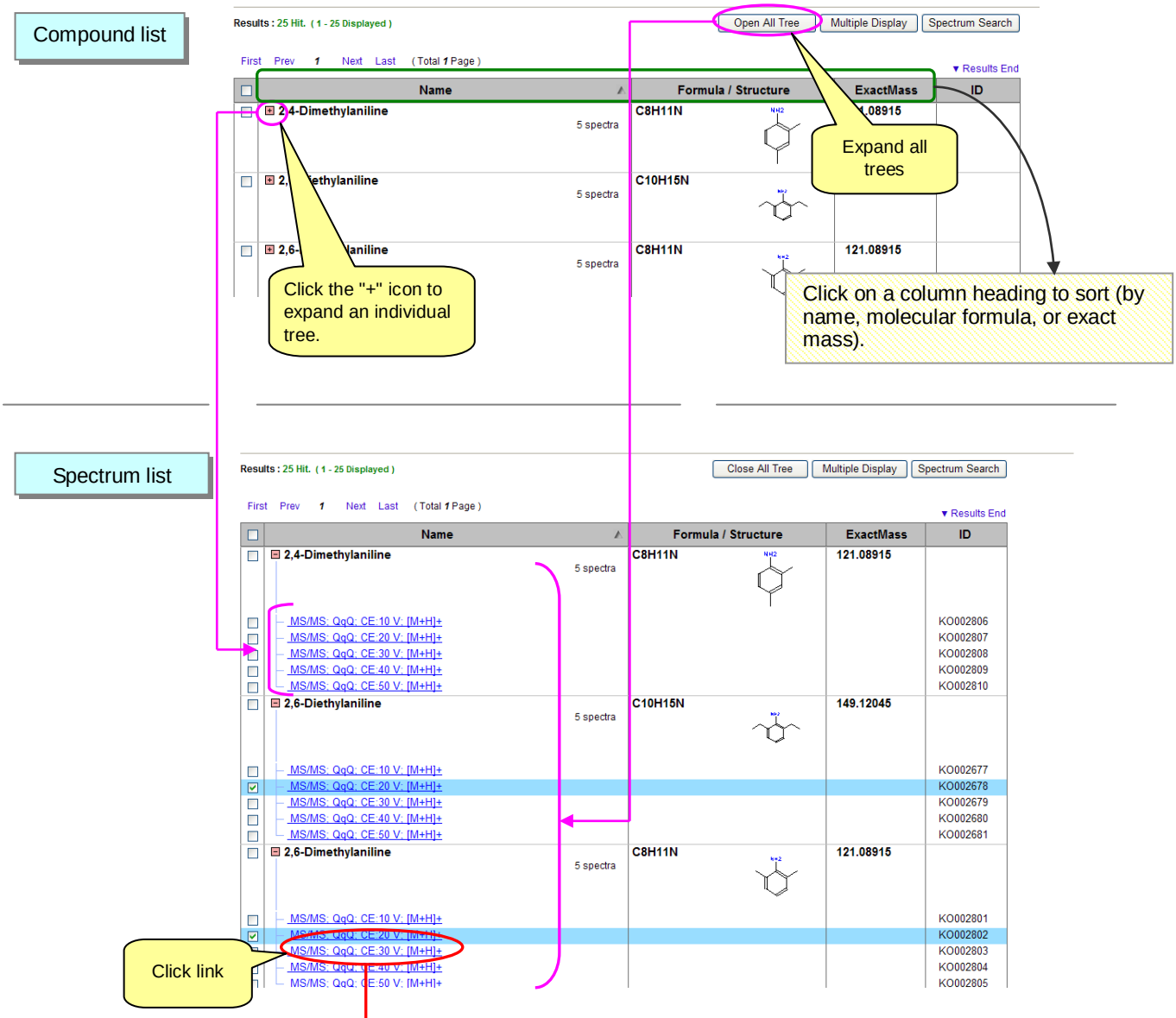
6. Others

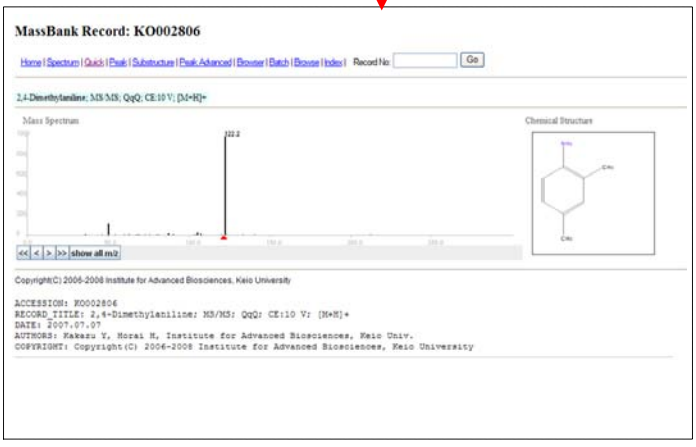
6.1 Search Results

When you conduct a search via "Quick Search", "Substructure Search", "Peak Search", "Peak Search Advanced", or "Record Index" , the search results are displayed in a common format.

<<Operation 1>>

List of Search Results




MassBank Record: KO002806
ACCESSION: KO002806
RECORD_TITLE: 2,4-Dimethylaniline; MS/MS; QqQ; CE:10 V; [M+H]+
DATE: 2007.07.07
COPYRIGHT: Copyright (C) 2006-2008 Institute for Advanced Biosciences, Keio University

MassBank record of an individual spectral data is displayed.

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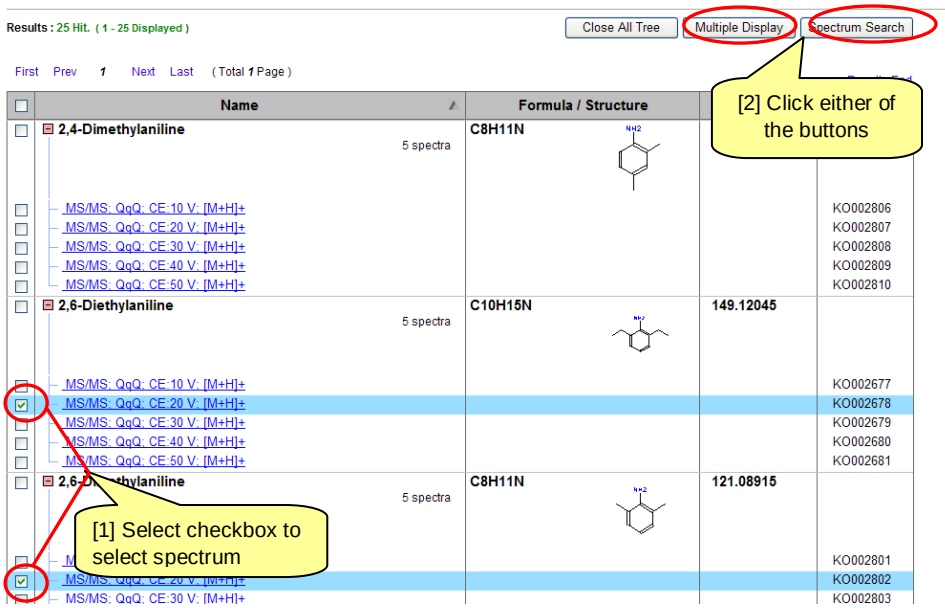
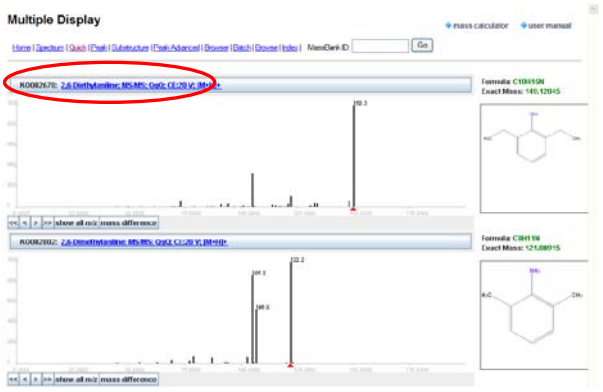
<<Operation 2>>

Interaction with "Multiple Display" and "Spectrum Search"

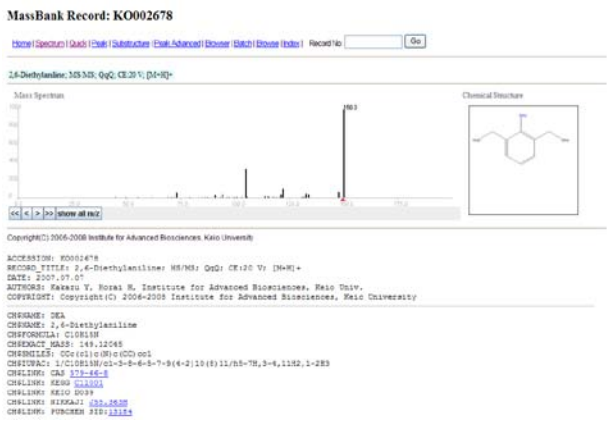


Clicking "Show Spectra"

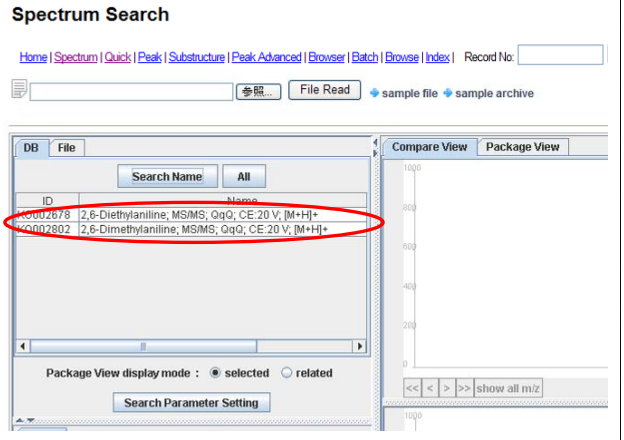


The selected spectra are displayed in tiled view.

Click a button displaying a record title to show the MassBank record.

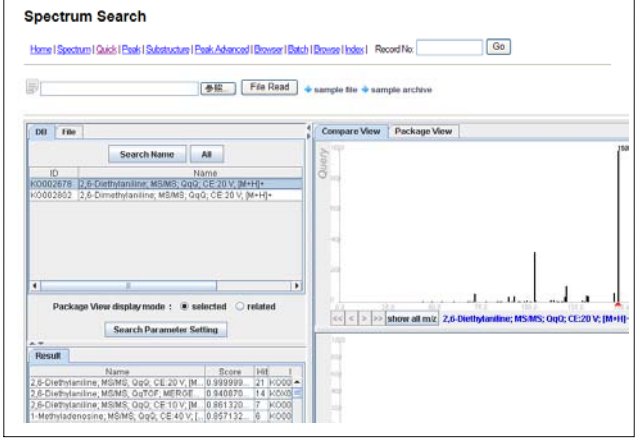


Clicking "Spectrum Search"



The "Spectrum Search" page opens, and the selected spectra are added to the query.

You can search with the selected spectrum as the query.



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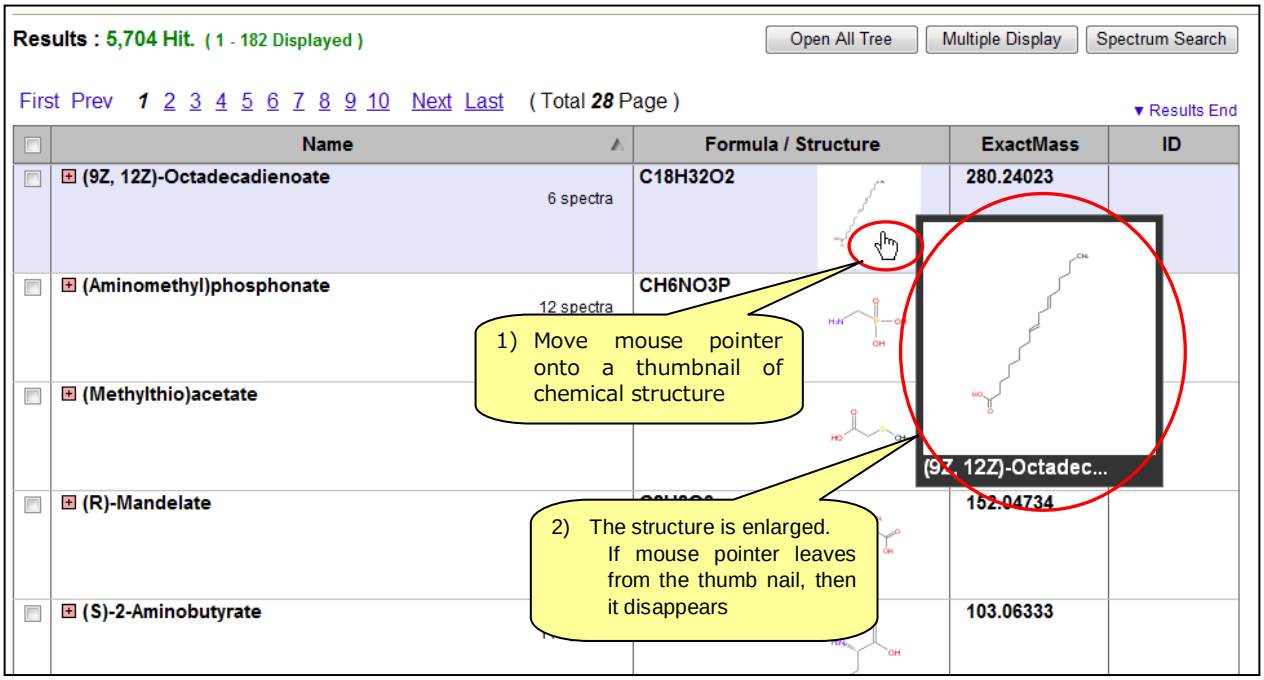
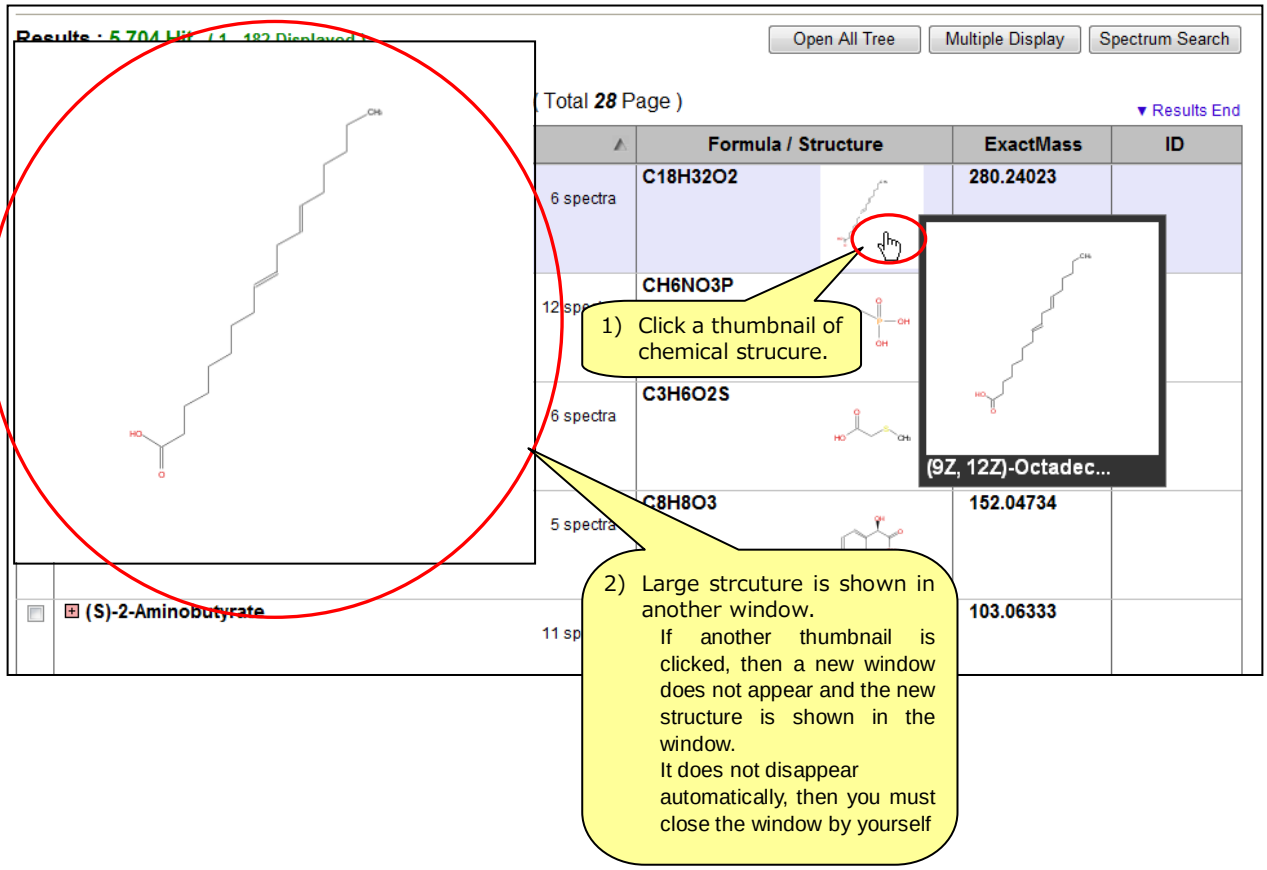
<<Operation 3>>

Brief display of chemical structure





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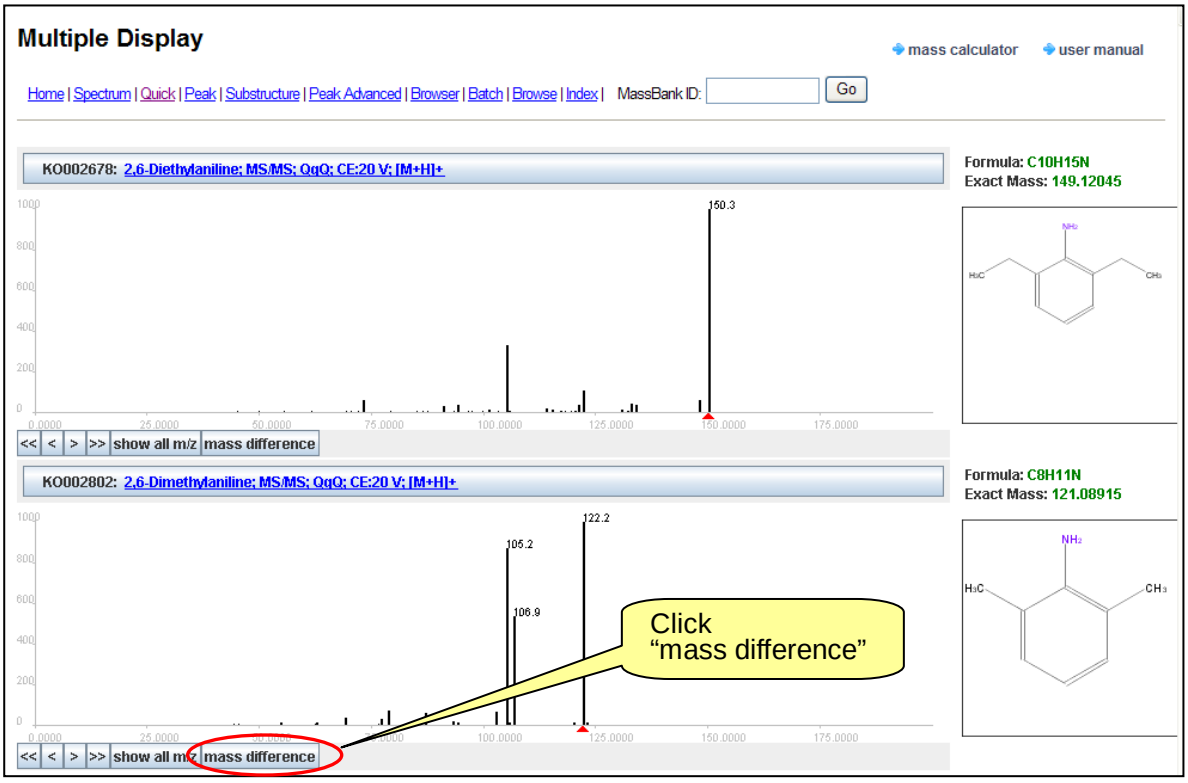
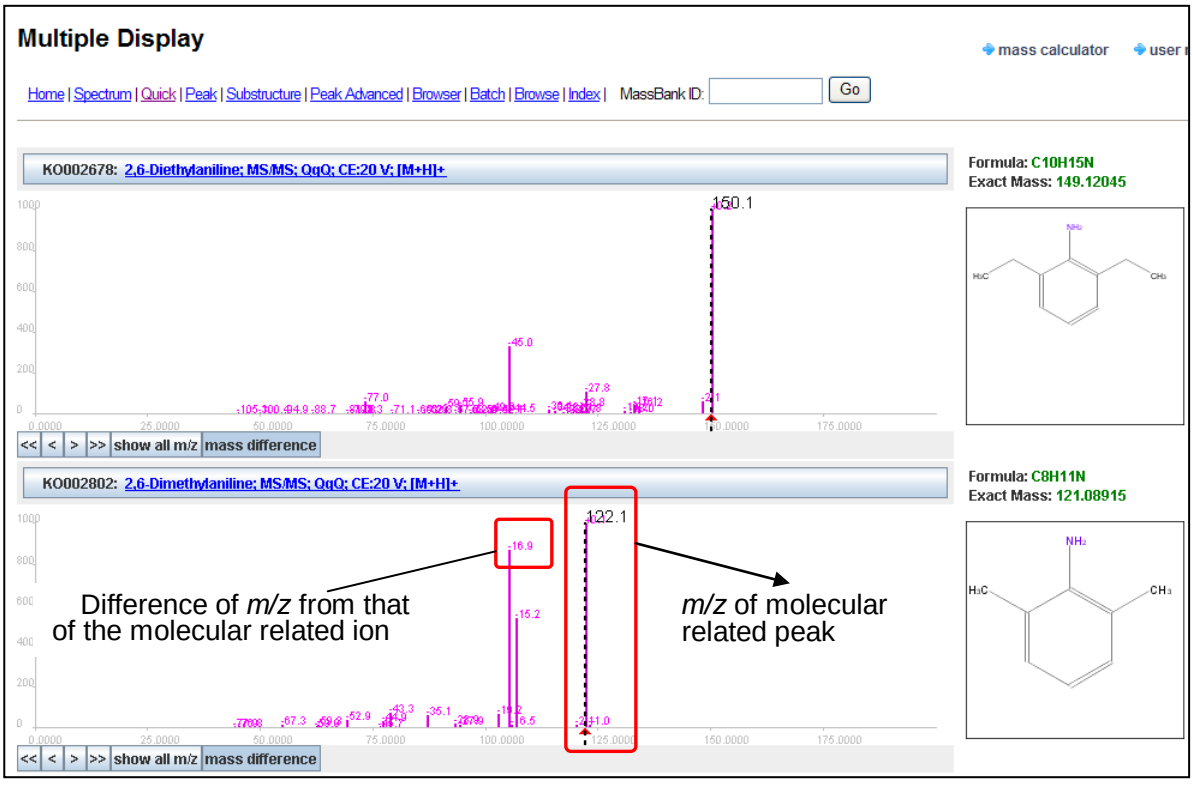
>> mass difference

When click the "mass difference" button on the "Multiple Display" panel of "Compound and Peak Search Results", spectra display the peaks with the value of *m/z* difference from that of the molecular related ion.


Multiple Display
mass calculator
user manual
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | MassBank ID: Go
KO002678: 2,6-Diethylaniline; MS/MS; QqQ; CE:20 V; [M+H]+
Formula: C10H15N
Exact Mass: 149.12045
150.3
<< < > >> show all m/z mass difference
KO002802: 2,6-Dimethylaniline; MS/MS; QqQ; CE:20 V; [M+H]+
Formula: C8H11N
Exact Mass: 121.08915
122.2
105.2
106.9
Click
"mass difference"
<< < > >> show all m/z mass difference


Multiple Display
mass calculator
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | MassBank ID: Go
KO002678: 2,6-Diethylaniline; MS/MS; QqQ; CE:20 V; [M+H]+
Formula: C10H15N
Exact Mass: 149.12045
150.1
<< < > >> show all m/z mass difference
KO002802: 2,6-Dimethylaniline; MS/MS; QqQ; CE:20 V; [M+H]+
Formula: C8H11N
Exact Mass: 121.08915
122.1
16.9
15.2
Difference of *m/z* from that of the molecular related ion
m/z of molecular related peak
<< < > >> show all m/z mass difference

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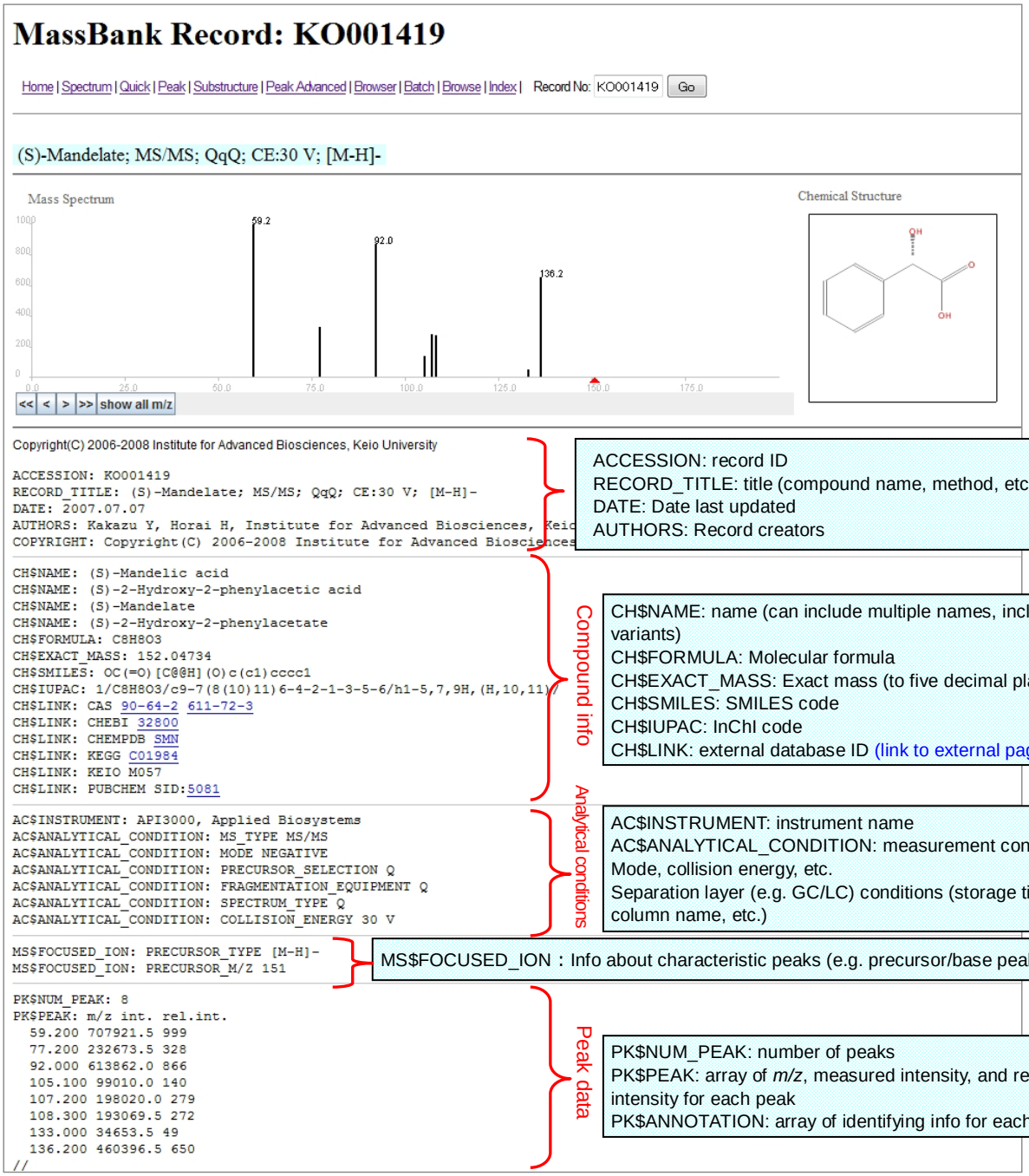
6.2 MassBank Record Detailed Display

The MassBank record is the fundamental unit of data in the MassBank database. Each mass spectrum has one MassBank record. In addition to peak data, each record includes the compound information (CH$), test conditions (AC$), etc. (To see "Record Editor Manual" for more details)


MassBank Record: KO001419
Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No: KO001419 Go
(S)-Mandelate; MS/MS; QqQ; CE:30 V; [M-H]-
Mass Spectrum
Chemical Structure
59.2
92.0
136.2
<< < > >> show all m/z
Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University
ACCESSION: KO001419
RECORD_TITLE: (S)-Mandelate; MS/MS; QqQ; CE:30 V; [M-H]-
DATE: 2007.07.07
AUTHORS: Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio
COPYRIGHT: Copyright(C) 2006-2008 Institute for Advanced Biosciences
CH$NAME: (S)-Mandelic acid
CH$NAME: (S)-2-Hydroxy-2-phenylacetic acid
CH$NAME: (S)-Mandelate
CH$NAME: (S)-2-Hydroxy-2-phenylacetate
CH$FORMULA: C8H8O3
CH$EXACT_MASS: 152.04734
CH$SMILES: OC(=O)[C@@H](O)c(c1)cccc1
CH$IUPAC: 1/C8H8O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7,9H,(H,10,11)/
CH$LINK: CAS 90-64-2 611-72-3
CH$LINK: CHEBI 32800
CH$LINK: CHEMPDB SMN
CH$LINK: KEGG C01984
CH$LINK: KEIO M057
CH$LINK: PUBCHEM SID:5081
AC$INSTRUMENT: API3000, Applied Biosystems
AC$ANALYTICAL_CONDITION: MS_TYPE MS/MS
AC$ANALYTICAL_CONDITION: MODE NEGATIVE
AC$ANALYTICAL_CONDITION: PRECURSOR_SELECTION Q
AC$ANALYTICAL_CONDITION: FRAGMENTATION_EQUIPMENT Q
AC$ANALYTICAL_CONDITION: SPECTRUM_TYPE Q
AC$ANALYTICAL_CONDITION: COLLISION_ENERGY 30 V
MS$FOCUSED_ION: PRECURSOR_TYPE [M-H]-
MS$FOCUSED_ION: PRECURSOR_M/Z 151
PK$NUM_PEAK: 8
PK$PEAK: m/z int. rel.int.
59.200 707921.5 999
77.200 232673.5 328
92.000 613862.0 866
105.100 99010.0 140
107.200 198020.0 279
108.300 193069.5 272
133.000 34653.5 49
136.200 460396.5 650
//
ACCESSION: record ID
RECORD_TITLE: title (compound name, method, etc.)
DATE: Date last updated
AUTHORS: Record creators
Compound info
CH$NAME: name (can include multiple names, including variants)
CH$FORMULA: Molecular formula
CH$EXACT_MASS: Exact mass (to five decimal places)
CH$SMILES: SMILES code
CH$IUPAC: InChI code
CH$LINK: external database ID (link to external page)
Analytical conditions
AC$INSTRUMENT: instrument name
AC$ANALYTICAL_CONDITION: measurement conditions
Mode, collision energy, etc.
Separation layer (e.g. GC/LC) conditions (storage time, column name, etc.)
MS$FOCUSED_ION : Info about characteristic peaks (e.g. precursor/base peak)
Peak data
PK$NUM_PEAK: number of peaks
PK$PEAK: array of m/z, measured intensity, and relative intensity for each peak
PK$ANNOTATION: array of identifying info for each peak

∗For details of MassBank Record, see "Record Editor Manual".

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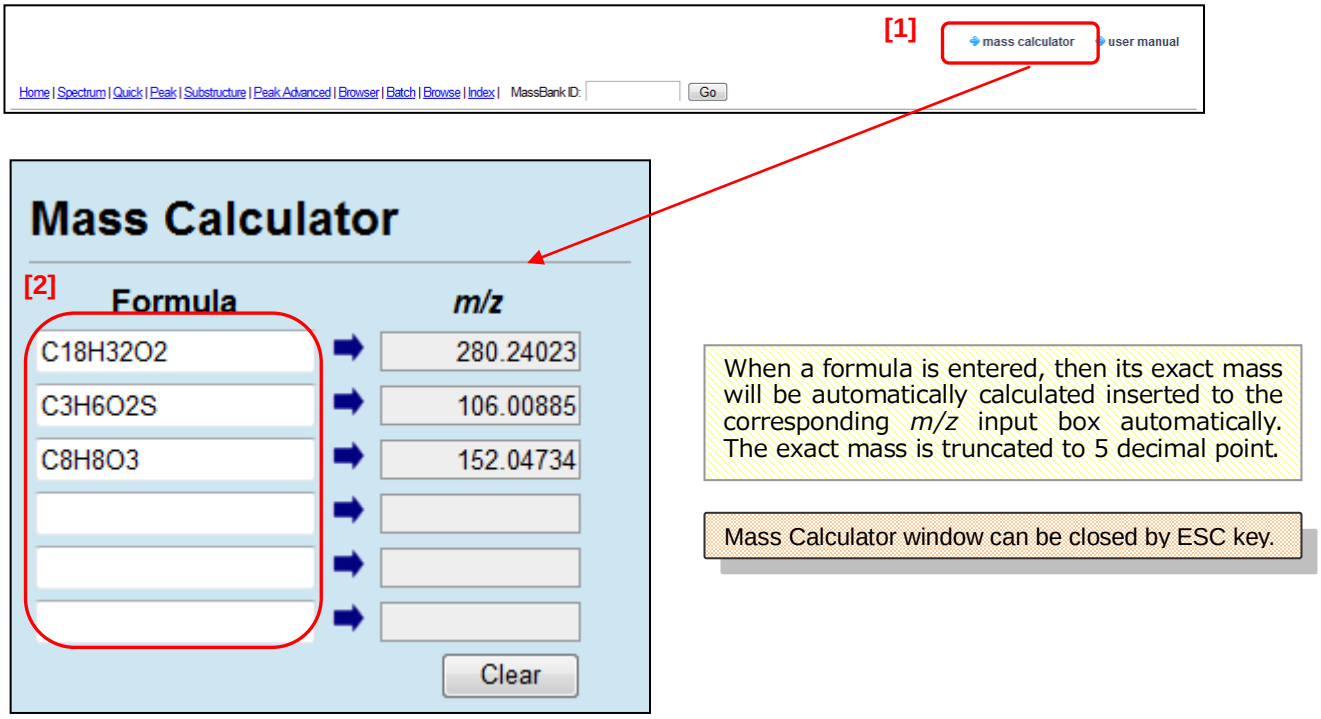
6.3 Basic Mass Calculation Tool

Mass Calculator is a basic mass calculation tool that you can use everywhere in MassBank. It is placed at the upper right corner of every search pages. It calculate *m/z* (*i.e.* exact mass) of input formula automatically.



When a formula is entered, then its exact mass will be automatically calculated inserted to the corresponding *m/z* input box automatically. The exact mass is truncated to 5 decimal point.

Mass Calculator window can be closed by ESC key.

[1] Click "mass calculator"

MassCalculator appears in a separate window.

[2] Input Formula

When a formula is entered, then *m/z* is automatically calculated.

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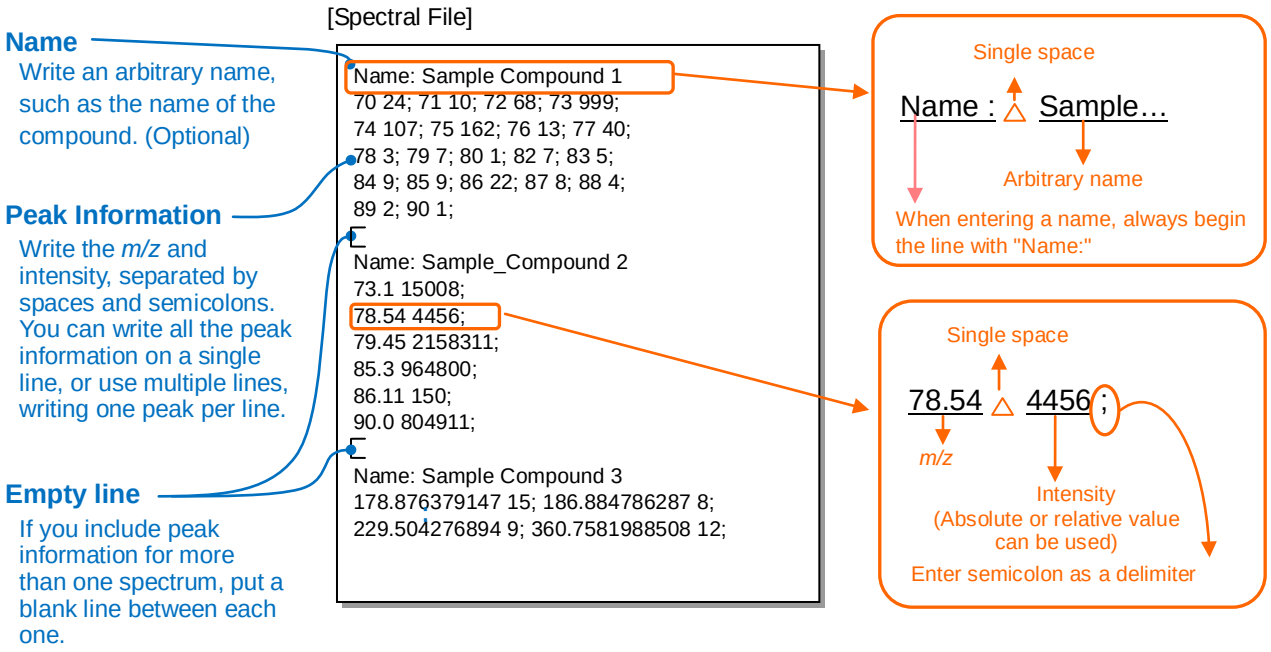
6.4 Comparison Tool of User Spectra

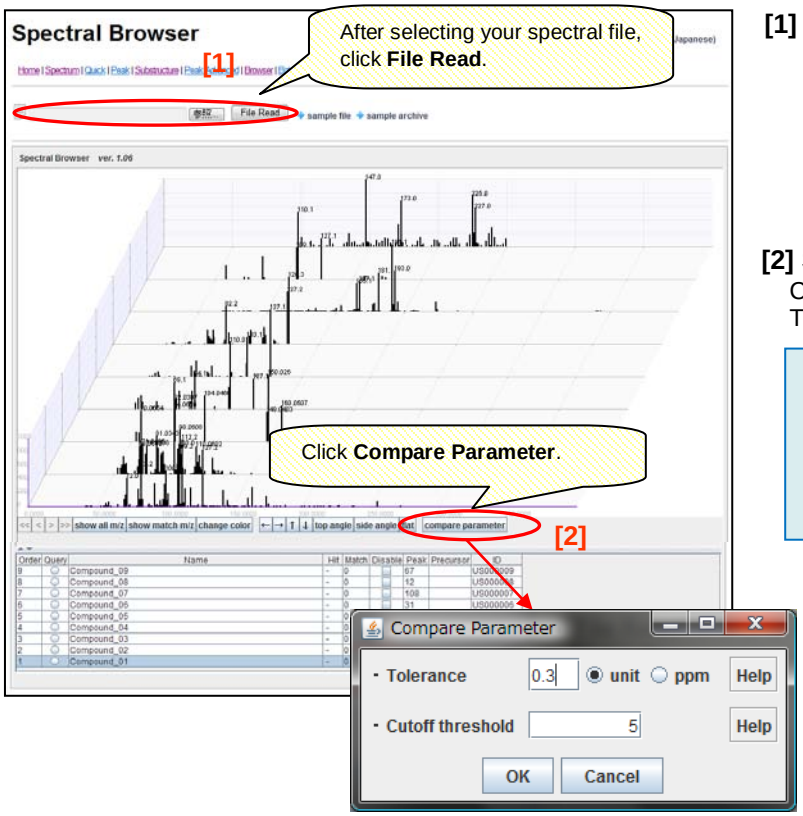
Spectral Browser is a comparison tool of spectra which reads a file which consists of a set of user spectra and displays them in perspective drawing. The upper limit of user spectra is 20. It also compare input spectra each other.

(1) Prepare the spectral file

The format of an input of Spectral Browswer, so-called a spectral file, is as follows. You can download a sample from http://www.massbank.jp/sample/sample.zip . The format of this spectral file is same as the format of a query file of Spectrum Search, then a spectral file is commonly used in Spectrum Search、Spectral Browser.


[Spectral File]
Name
Write an arbitrary name, such as the name of the compound. (Optional)
Peak Information
Write the m/z and intensity, separated by spaces and semicolons. You can write all the peak information on a single line, or use multiple lines, writing one peak per line.
Empty line
If you include peak information for more than one spectrum, put a blank line between each one.
Name: Sample Compound 1
70 24; 71 10; 72 68; 73 999;
74 107; 75 162; 76 13; 77 40;
78 3; 79 7; 80 1; 82 7; 83 5;
84 9; 85 9; 86 22; 87 8; 88 4;
89 2; 90 1;
Name: Sample_Compound 2
73.1 15008;
78.54 4456;
79.45 2158311;
85.3 964800;
86.11 150;
90.0 804911;
Name: Sample Compound 3
178.876379147 15; 186.884786287 8;
229.504276894 9; 360.7581988508 12;
Single space
Name : Sample…
Arbitrary name
When entering a name, always begin the line with "Name:"
Single space
78.54 4456 ;
m/z
Intensity
(Absolute or relative value can be used)
Enter semicolon as a delimiter

(2) Load spectral file and set the compare parameters



Compare Parameter Setting Window

[1] Load the spectral file

Click **"Browse"**, and select a spectral file. Afterwards, click **"File Read"**, then Spectral Browser reads the spectral file and display the spectra in it

[2] Set the compare parameters

Click **Compare Parameter**.
The Setting window opens.

Settings
- **Tolerance**:
  m/z error range
- **Cutoff Threshold**:
  Relative intensity threshold

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(3) Perform the compare

When you specify an arbitrary spectrum as a query, then you can compare input spectra in one-to-many manner.

[1] Select query spectrum

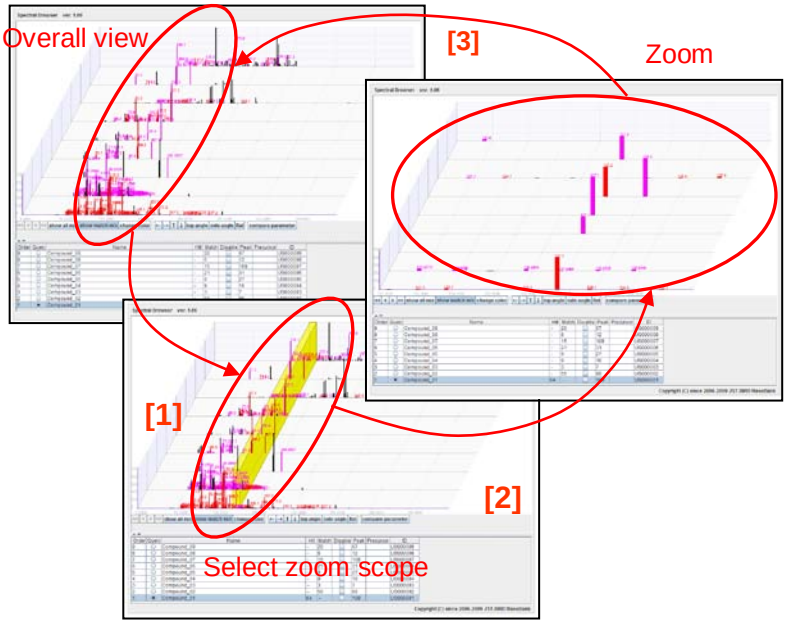
Click a radio button for selecting a query. The one-to-many comparison is suddenly executed and its results are reflected automatically.

Peak Color in Spectrum Comparison Window

In the spectrum comparison windows in Compare View and Package View, matching peaks can be distinguished by color.

Matching m/z on query peak / *Peak*	Perfect Match	Match within Error Margin
Query Spectrum	**Red**	**Red**
Retrieved Spectrum	**Red**	**Pink**

<<Handy Feature 1: Spectrum Zoom>>



[1] Select location to zoom

Drag from the location of the start of the zoom.

[2] Set zoom position

Drop to set the location on the spectrum to zoom.

[3] End zoom

Double click in comparison window, then return to the initial size without zooming

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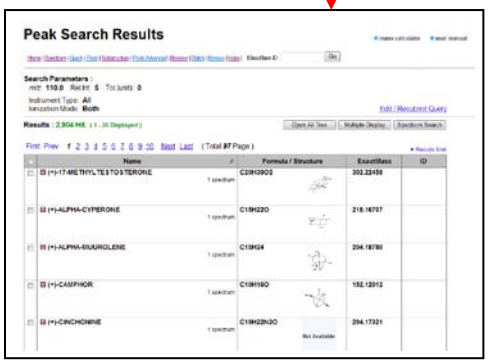
<< Handy Feature 2: Peak Manipulation>>



Peak Search Results Window

a Highlight peak

Place the cursor over a peak. It is highlighted in blue, and the *m/z* and intensity values appear.

b Select peak

Click on a desired peak. It is rendered in blue to indicate that it is selected. Up to 6 peaks can be selected.

Peak Rendering Color
Highlighted: Blue
Selected: Light blue

c Search for peaks

If you right click while one or more peaks are selected, a menu appears, and **"Peak Search"** can be selected. The peak search begins immediately after selection.

d Cancel peak selection

Select **"Select Reset"** from a menu popped up by a right button click in graphic area.

- Highlight & select peak in Spectral Browser -
In Spectral Browser, when you highlight or select a peak in a spectrum, peaks in other spectra are also highlighted or selected if whose *m/z* are completely equal to the *m/z* of the highlighted/selected peak.

<< Handy Feature 3: Spectrum Manipulation>>

Spectrum Manipulation Buttons

<<, <, >, >>
... Move display location (only when zoomed on spectrum

show all m/z
… Display *m/z* values of all peaks

show match m/z
… Display m/z values of matching peaks

change color
… Change color of entire spectrum

←, →, ↑, ↓
… Change angle (manual manipulation)

top angle
… Change angle (top perspective)

side angle
… Change angle (side perspective)

flat
… Change angle (all spectrums in flat view)

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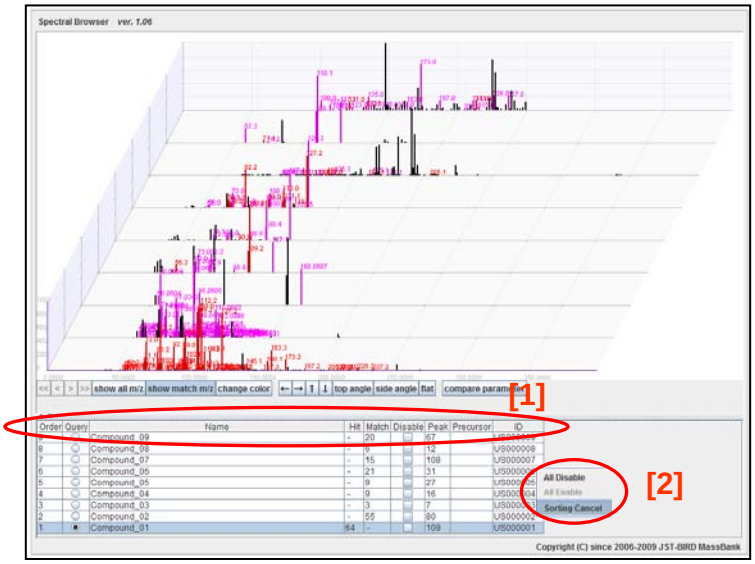
<< Handy Feature 4: Sort Spectra>>



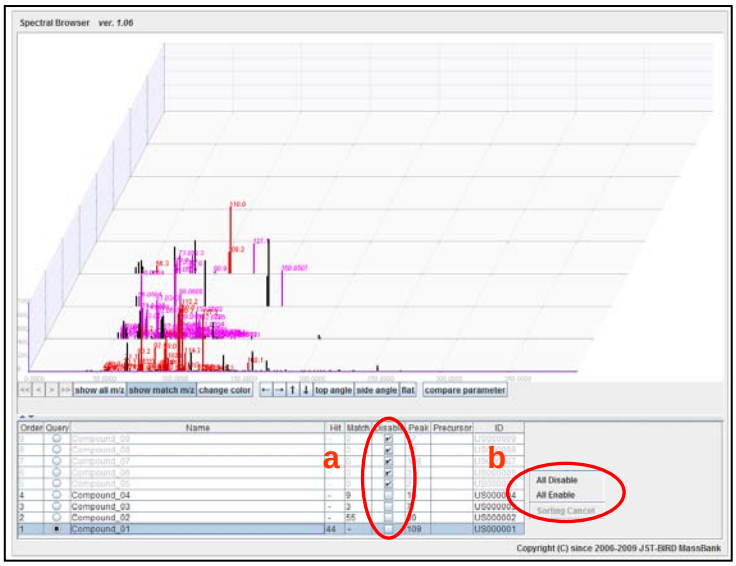
[1] Sort Spectra

Click one of header items in comparison list (*i.e.* **"Order"**, "**Query**", **"Name", "Hit", "Match", "Disable",** "**Peak", "Precusor",** and **"ID"**), then the list is sorted by the item. Consecutive clicks of an item change the order of sorting cyclically in ascending, descending and without sorting

[2] Cancel sorting

Select **"Sorting Cancel"** in a menu popped up by right button click on comparison list.

<< Handy Feature 5: Spectrum Hiding>>



a Hide/show specrum

For each item in comparison list, tick its checkbox "**Disable**", then the corresponding spectrum is hided. Untick the checkbox, then it appears again

b Hide/show all spectra

Select "**All Disable**" in a menu popped up by right button click on comparison list, then all spectra are hided. Select "**All Enable**" in the same menu, then all spectra appear again.

- Comparison window and comparison list -

Comparison window and Comparison list are operated simultaneously. For example, spectra are sorted in comparison list, the results is suddenly reflected to comparison window and spectra in comparison window are also sorted in same order.

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Contact

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